US High Production Volume Chemical Program

Category Summary

For

Fuel Oils Category

Prepared by:

Olefins Panel of the American Chemistry Council

March 28, 2005

EXECUTIVE SUMMARY

The Olefins Panel of the American Chemistry Council (ACC) hereby submits the category summary report for the Fuel Oils Category under the Environmental Protection Agency's High Production Volume (HPV) Chemical Challenge Program (Program). The purpose of this report is to:

- Present results of an assessment to determine whether 8 production streams can be adequately characterized with existing data (this includes data developed as described in the Fuel Oils HPV test plan).
- Summarize the SIDS (Screening Information Data Set) physicochemical, environmental fate and effects, and human health HPV Program endpoints for the Fuel Oils Category.
- Provide a description of manufacturing processes, potential exposure sources, and uses for Fuel Oils.

The Fuel Oils Category contains 8 streams:

- Heavy Pyrolysis Fuel Oil
- Quench Oil from water quench
- Light Pyrolysis Fuel Oil
- Pyrolysis C10+ Fuel Oil
- Combined Fuel Oil (E&P, from the ethylene process and pyrolysis gasoline units)
- Hydrotreated Flux Oil
- Biphenyl Concentrate
- Combined Fuel Oil (B&P, from benzene HDA and pyrolysis gasoline units)

After all data were evaluated to determine whether the streams formed a cohesive category, it was decided that they can be considered a category. The following category report summarizes HPV Program data for the Fuel Oils Category.

A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. Biphenyl Concentrate, one of the streams, can be relatively pure, containing up to 95% biphenyl (the reported range is 65 to 95%). The Chemical Abstracts Service (CAS) registration numbers (RNs) used to represent the 8 streams are generally vague with respect to the specifics that distinguish the streams within the category. Therefore, more than one CAS RN may correctly represent a single stream and a CAS RN may be applicable to more than one stream. For this reason, this category was evaluated based on 8 compositionally differentiated process streams, rather than on the CAS RNs in this category.

Exposure

The Fuel Oils Category includes 8 commercial product streams from the Olefins Industry. The category streams are complex mixtures of variable composition and consist of the high molecular weight (generally carbon number 10 and higher) hydrocarbons produced by the olefins manufacturing processes. The primary use of the category streams is as blending streams for production of industrial or marine fuel oil. The streams are also used in limited cases for production of industrial heat transfer fluids or production of carbon black. The streams are sometimes used as fuel on site where they were produced. Thirteen CAS RNs are used to represent these streams.

There are no known or expected applications that would result in consumer exposure for these materials.

The category streams are transported for use to other industrial facilities in bulk by barge, pipeline, tank car, or tank truck.

Inhalation is the likeliest route of potential exposure although the volatility of the hydrocarbon components that make up the streams is low. Other possible exposure routes include dermal exposures (from spills). A potential, but very unlikely route of exposure is oral exposures (from contaminated ground water).

Occupational exposure is limited because production and use of these streams is generally in closed systems, and because of the low vapor pressure of the streams. The Occupational Safety and Health Administration (OSHA) Permissible Exposure Limits (PELs) and the American Conference for Governmental Industrial Hygienists (ACGIH) Threshold Limit Values (TLVs) apply to some of the components in the category streams (naphthalene, biphenyl, dicyclopentadiene, and indene) and compliance with these occupational exposure limits should reduce or eliminate potential occupational exposure to these streams.

Environmental exposure is limited since emissions from production and use are limited and controlled by a number of volatile organic compound and hazardous air pollutant environmental regulations at both the federal and state level.

Human Health

Existing *in vivo and in vitro* data are sufficient to characterize the human health hazards of substances included in the Fuel Oils Category for purposes of the HPV Program. From data on representative streams, and read-across from streams of similar composition, it can be concluded that Fuel Oils Category streams are not acutely toxic by the oral, dermal or inhalation routes of exposure. Streams in the Fuel Oils Category are likely to be irritating to the skin and eyes.

Data are available to adequately characterize the repeated dose toxicity of the Fuel Oils Category. The most consistent observations among these rodent studies were decreased body weight and alterations in certain clinical chemistry and haematology parameters.

Adequate data are available to characterize the teratogenic, reproductive, and developmental toxicity potential of Fuel Oils Category streams. In these rodent studies no developmental or reproductive toxicity was observed at doses that were not maternally toxic. Systemic effects were observed in parental animals including reduced body weight gain and increased clinical observations. Based on available data, Fuel Oils Category streams are unlikely to induce teratogenic, reproductive or developmental toxicity.

Adequate data are available from in vitro and in vivo rodent studies to characterize the genotoxic potential of Fuel Oils Category streams. The results of a diverse array of mutagenicity, transformation, and clastogenicity assays indicate positive responses in some assays and negative responses in others. Light Pyrolysis Fuel Oil, Heavy Pyrolysis Oil and Biphenyl Feedstock demonstrated activity in assays for general genetic damage (unscheduled DNA synthesis and sister chromatid exchange), but were inactive in assays for mutagenicity (HGPRT and Ames assays), clastogenicity (micronucleus) and cell transformation. Aromatic Pyrolysis Oil was determined to be mutagenic and clastogenic, induced DNA synthesis (indication of repair) and produced transformation in culture cells. EDS Experimental Fuel Oil was mutagenic in the Ames assay and transformed Syrian hamster embryo cells in culture. Mutagenic activity required metabolic activation. Using Aromatic Pyrolysis Oil as a worst case surrogate for the Fuel Oils Category, it is concluded that these streams are genotoxic.

Adequate data are available to characterize the carcinogenic potential of Fuel Oils Category streams. Pyrolysis Fuel Oil was carcinogenic in the mouse skin painting bioassay. Although the method used a qualitative procedure of skin painting rather than exact volume application, and the material was not analyzed, the results were unambiguous. The described process conditions and the benzo(a)pyrene levels (300-500 ppm) were consistent with a dermal carcinogenic response and the latency period was short enough to anticipate possible metastatic spread.

While the study was limited in the details reported and did not include information on presence and degree of irritation, other studies clearly indicate that the materials in this category are irritating to skin. Therefore, the possibility that the effects reported are due at least in part to chronic irritation of the skin can not be eliminated.

Environment

Results of distribution modeling show that constituents of streams in the Fuel Oils Category will partition largely between the air, water, and soil compartments, with a negligible amount partitioning to sediment. Volatilization to the air can contribute to the loss of some constituents from aqueous and terrestrial habitats. Although some constituents have a moderate degree of water solubility, wet deposition of category constituents is not likely to play a significant role in their atmospheric fate because they rapidly photodegrade. In the air, these constituents have the potential to rapidly degrade through indirect photolytic processes mediated primarily by hydroxyl radicals with calculated degradation half-lives ranging from 1.1 to 53.0 hours, depending on hydroxyl radical concentration. Aqueous photolysis and hydrolysis will not contribute to the transformation of category constituents in aquatic environments because they are either poorly soluble or not susceptible to these reactions. Streams in this category are subject to biodegradative processes. Two category streams, Heavy Pyrolysis Fuel Oil and Pyrolysis C10+ Fuel Oil, and one analog stream, 1,1'-biphenyl, exhibited a range 7 to 57% biodegradation under standard testing procedures after 28 days. The remaining streams that were not tested are expected to demonstrate a similar range of biodegradability.

Aquatic toxicity testing results for two different complex streams, Heavy Pyrolysis Fuel Oil and Pyrolysis C10+ Fuel Oil, suggest that category members will exhibit a moderate order of toxicity. The effect values for the two streams fell within a relatively narrow range. The two streams combined contain constituents shared by the remainder of the streams within this category, and therefore justifies their use to characterize the potential effects of the untested streams.

The 96-hour LC_{50} and LL_{50} results for *Oncorhynchus mykiss* (rainbow trout) range between 1.0 to 4.4 and 1.1 to 5.6 mg/L, respectively. The 48-hour EC_{50} and EL_{50} results for *Daphnia magna* (invertebrate) range between 1.2 to 2.7 and 1.2 to 3.3 mg/L, respectively. The 96-hour EC_{50} and EL_{50} results based on biomass and growth rate for *Pseudokirchneriella subcapitata* (green alga) range from 0.9 to 1.6 and 1.2 to 2.2 mg/L, respectively, while the 96-hour NOEC and NOELR results based on biomass and growth rate range between 0.12 to 0.42 and 0.18 to 0.39 mg/L, respectively. Fish acute toxicity data (96-hour LL_{50}) for two marine species that were developed with an analog substance and only reported as lethal loading values were 3.2 and 56.0 mg/L. A second analog substance tested in an acute *Daphnia magna* study exhibited a 48-hour EL_{50} = 23.6 mg/L. Untested streams are expected to exhibit toxicities within the range of values demonstrated by these data.

Conclusion

The extensive body of data available for mammalian and environmental endpoints on category streams in this category and analog substances are sufficient to fully characterize the potential toxicity of category members for purposes of the US HPV Program and to demonstrate the integrity of the category.

OLEFINS PANEL of the AMERICAN CHEMISTRY COUNCIL
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* Companies that are part of the Olefins Panel, but do not produce products in the Fuel Oils Category.

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1 CATEGORY DESCRIPTION AND JUSTIFICATION

1.1 Category Identification

For purposes of the US High Production Volume (HPV) Chemical Challenge Program (Program), the Fuel Oils Category test plan submitted in September 2003 (Olefins Panel, HPV Implementation Task Group, 2003) included 8 production streams[1] and 12 Chemical Abstracts Service (CAS) registration numbers (RNs) (Table 1). Since the time the test plan was submitted, 1 CAS RN, 64742-47-8, has been added to the Hydrotreated Flux Oil stream, bringing to a total, 13 CAS RNs covered under this category (Table 1).

The test plan identified existing data based on an extensive technical review of the category to adequately characterize the 8 streams for the HPV Program endpoints. Additional data were also developed as described in the test plan. After consideration of all data, it was decided that the following data would be adequate to characterize the streams in this category:

- Data as described in robust summaries submitted with the Olefins Panel, HPV Implementation Task Group, HPV Chemical Challenge Program test plan for the Fuel Oils Category (Olefins Panel, 2003).
- Data submitted by the Olefins Panel, HPV Implementation Task Group in the form of robust summaries to support the Fuel Oils Category [submitted to the US Environmental Protection Agency (USEPA) in February, 2004].
- New data developed for two streams, Heavy Pyrolysis Fuel Oil and Pyrolysis (C10+) Fuel Oil, by the Olefins Panel, HPV Implementation Task Group (robust summaries for these studies are submitted with this category summary report).

After all data were evaluated to determine whether the streams formed a cohesive category, it was decided that they can be considered a category. The following category report summarizes HPV Program data for the Fuel Oils Category.

[1] A production stream is a mixture of chemicals that arises from a chemical reaction or separation activity.

Table 1. Production Streams, CAS RNs, and CAS RN Names in the Fuel Oils Category

Production Streams	CAS RN	CAS RN Name[1]
Heavy Pyrolysis Fuel Oil	68513-69-9	Residues, petroleum, steam-cracked light
	64741-62-4	Clarified oils, petroleum, catalytic cracked
	69013-21-4	Fuel oil, pyrolysis
	8002-05-9	Petroleum
Quench Oil (from the ethylene process unit water quench system)	68513-69-9	Residues, petroleum, steam-cracked light
	69430-33-7	Hydrocarbons, C6-30
Light Pyrolysis Fuel Oil (from the ethylene process unit)	68475-80-9	Distillates, petroleum, light steam-cracked naphtha
	68514-34-1	Hydrocarbons, C9-14, ethylene-manufacturing-by-product
	68527-18-4[2]	Gas oils, petroleum, steam-cracked
Pyrolysis C10+ Fuel Oil (from pyrolysis gasoline distillation)	68513-69-9	Residues, petroleum, steam-cracked light
	68921-67-5	Hydrocarbons, ethylene-manuf.-by-product distillation residues
Combined Fuel Oil (E&P) (from the ethylene process and pyrolysis gasoline units)	64742-90-1	Residues, petroleum, steam-cracked
	68131-05-5	Hydrocarbon oils, process blends
	68527-18-4	Gas oils, petroleum, steam-cracked
	69013-21-4	Fuel oil, pyrolysis
Hydrotreated Flux Oil	64742-47-8[3]	Distillates, petroleum, hydrotreated light
	69013-21-4	Fuel oil, pyrolysis
Biphenyl Concentrate	68409-73-4	Aromatic hydrocarbons, biphenyl-rich
Combined Fuel Oil (B&P) (from benzene HDA and pyrolysis gasoline units)	68513-69-9	Residues, petroleum, steam-cracked light

1 The definitions found in the TSCA (Toxic Substances Control Act) Chemical Substance Inventory for the CAS RNs in this category are vague with respect to composition. Therefore, it is not uncommon to find that one CAS RN is correctly used to describe different streams (different compositions) or that two or more CAS RNs are used to describe one stream (similar composition).

2 This CAS RN is currently used with the Combined Fuel Oil stream. However, it was previously used with the Light Pyrolysis Fuel Oil stream and test data are identified for this stream and CAS RN.

3 This CAS RN was not included in the original list of CAS RNs sponsored in this category. It has been added to this category summary report because it is an additional CAS RN that may be used to represent the Hydrotreated Flux Oil stream.

The streams in this category include hydrocarbon reaction products with a carbon (C) number distribution that is predominantly between C7 to C13 and a significant level of aromatics and olefins. The typical composition of streams in this category is shown in Table 2.

Table 2. Typical Constituent (wt%) Range in Streams of the Fuel Oils Category

Constituent	Fuel Oil (FO) Stream Number and Name							
	FO 1	FO 2	FO 3	FO 4	FO 5	FO 6	FO 7	FO 8
	Heavy Pyrolysis Fuel Oil from the Ethylene Process Unit* (wt %)	Quench Oil from the Ethylene Process Unit Water Quench System (wt %)	Light Pyrolysis Fuel Oil from the Ethylene Process Unit (wt %)	Pyrolysis C10+ Fuel Oil from Pyrolysis Gasoline (wt %)	Combined Fuel Oil from Ethylene & Pyrolysis Gasoline (wt %)	Hydro-treated Flux Oil (wt %)	Biphenyl Concen-trate (wt %)	Combined Fuel Oil from Benzene HDA & Pyrolysis Fuel Oils (wt %)
1,3-Butadiene		0.1 - 0.3						
C6 Non-aromatics (NOS)					0.2 - 3.1			
C5s and Lighter (NOS)					1.8			
C6s and Lighter (NOS)								0.2
Benzene		0.1			0.2 – 4			0. 1 - 0.3
C7 Paraffins & Naphthenes					3			
Toluene		5			0.2 – 1.3		1 - 8	
C8 Paraffins & Naphthenes					6.1			
Ethylbenzene		5					1	
C8 Aromatics (NOS)					0.4 – 2.6			
Xylenes, Mixed		5					2	
Styrene		0 - 5			0.9			
C9 Aromatics (NOS)				2	12.6			
C9s (NOS)						<1		
Other Benzenes to Naphthalene					14.5			11
C9 Paraffins & Naphthenes					12.6			
C10+ (NOS)							3 – 25	
Trimethylbenzenes					1			
Dicyclopentadiene				20	0.9			7.5 - 11.7
C10 & C11 Codimers of C5 & C6 Olefins				30				
Indane (Indan)					1.5			
2,3-Benzindene					2 – 5			5 - 6.4
Methyl Dicyclopentadiene					0.9			
C10 Aromatics (NOS)					32.1			
C10s (NOS)						10		
C11s (NOS)						40		
C12s (NOS)						40		
C13s (NOS)						10		
Indene		5	5 – 15	2	0.7 - 0.8			3.8
Methyl Indenes					5.6			0.2 – 2
1,3-Diethyl-5-methylbenene					1.5			
Dimethylindan					4.0			
Dimethylindene					5.4			

Table 2. (continued)

Constituent	Fuel Oil (FO) Stream Number and Name							
	FO 1	FO 2	FO 3	FO 4	FO 5	FO 6	FO 7	FO 8
	Heavy Pyrolysis Fuel Oil from the Ethylene Process Unit* (wt %)	Quench Oil from the Ethylene Process Unit Water Quench System (wt %)	Light Pyrolysis Fuel Oil from the Ethylene Process Unit (wt %)	Pyrolysis C10+ Fuel Oil from Pyrolysis Gasoline (wt %)	Combined Fuel Oil from Ethylene & Pyrolysis Gasoline (wt %)	Hydro-treated Flux Oil (wt %)	Biphenyl Concen-trate (wt %)	Combined Fuel Oil from Benzene HDA & Pyrolysis Fuel Oils (wt %)
n-C13					1.3			
Methylcyclo-pentadiene Dimers					5.1			
Naphthalene		0.7 - 10	30 - 60	7	10 - 47		1 - 4	7 - 13.2
C7-C18 Cyclic Olefins (NOS)		65.0						
Methylnaphthalenes					3.8 - 30		1	
2-Methylnaphthalene				2				0.1 – 13
1-Methylnaphthalene				2				9
Fluoranthene		0 - 1.1						
1,1'-Biphenyl		0.5 - 5		6	1.1 - 5.1		65 - 95	25 - 34.6
Ethyl Naphthalene's					0.8			1.5 - 4
Substituted Naphthalenes				13				
1-Ethylnaphthalene				8				
Dimethylnaphthalenes				8	3.8			
Acenaphthylene		0.1 - 6.9						
Diphenylethane					2 – 7			
Acenaphthene		0.1 - 1.3						2
Fluorene					3			
C10 Paraffins & Naphthenes					1.1			
Phenanthrene					5			7
Anthracene		10			1 - 5			2
Heavy Hydrocarbons and Polycyclic Aromatics (NOS)				7.0				
Terphenyls								2.5
Methylbiphenyls					5 - 10		1 - 3	6.2
>C18 Cyclic Olefins (NOS)		5						
1,2-Dihydro-acenaphthylene				1				

NOS not otherwise specified

* Consists of C10+ and polycyclic aromatic hydrocarbons, NOS. Specific composition data were not available for the Heavy Pyrolysis Fuel Oil stream. This stream is expected to consist of the higher boiling polyaromatic and polycyclic hydrocarbon components (generally naphthalene and higher) that are included in the composition of the other category streams.

Note: The composition data shown are composites of reported values. The balances of these streams are expected to be other hydrocarbons that have boiling points in the ranges of the listed constituents. The composition limits indicted in the above table should not be considered to represent absolute limits for these streams. They represent the high and low reported values, and may be industry typical limit values.

The TSCA Chemical Substance Inventory definitions for the CAS RNs in this and in other categories from the Olefins Panel's HPV Program can be very general and vague with respect to

composition. Consequently, the data matrix for this category was developed based on 8 compositionally differentiated process streams, rather than on the CAS RNs in this category.

The Fuel Oils Category streams arise from production processes associated with ethylene manufacturing (see Appendix I for a description of the ethylene and associated processes). Briefly, descriptions of the 8 process streams are:

1. (FO 1) Heavy Pyrolysis Fuel Oil from the Ethylene Process Unit: In ethylene plants cracking liquid feedstocks, the cracking furnace effluent (after heat recovery) is further quenched by injection of recycled quench oil. This step results in the condensation of higher boiling hydrocarbon compounds that are typically separated from the rest of the furnace effluent as the bottoms of the primary fractionation tower or oil quench tower. Light hydrocarbons are stripped from the excess oils generated from this quench system, resulting in the stream identified here as heavy pyrolysis fuel oil consisting of C10+ and considerable PAHs.
2. (FO 2) Quench Oil from the Ethylene Process Unit Water Quench System: In ethylene plants cracking only gases, the cracking furnace effluent (after heat recovery) may be further quenched with water. This step results in the condensation of a relatively small amount of higher boiling hydrocarbon components that, after stripping to remove light hydrocarbons, may be isolated as the quench oils from of the ethylene process unit water quench system. This stream is predominantly C7 through components boiling at 650°F or higher. The reported composition indicates approximately 0.1 % benzene, 5% toluene, 12% C8 aromatics, 5% naphthalene, 10% anthracene, and 65% C7 to C18 cyclic olefins.
3. (FO 3) Light Pyrolysis Fuel Oil from the Ethylene Process Unit: In some cases, a light pyrolysis fuel oil is produced from the oil quench system in an ethylene plant that cracks liquid feedstocks. This stream may be produced as a side draw from the primary fractionation tower. The stream typically has a carbon number distribution of C9 to C14 and the major components are naphthalene (30 to 60%), methyl naphthalenes, and other substituted one and two ring aromatics.
4. (FO 4) Pyrolysis Fuel Oil from Pyrolysis Gasoline Distillation: This stream is separated by distillation from pyrolysis gasoline, as a bottoms product. The reported composition indicates a carbon number distribution of from C9 to hydrocarbons boiling at 650°F or higher. The reported typical composition includes approximately 20% dicyclopentadiene, 30% codimers of C5 and C6 monomers, and 20% naphthalene and substituted naphthalenes.
5. (FO 5) Combined Fuel Oil of the Ethylene Process and Pyrolysis Gasoline Units: A single combined fuel oil stream from the ethylene process unit and the pyrolysis gasoline unit is not an uncommon situation for the industry. The carbon number distribution for this stream is generally C10 to compounds with a boiling point of 650°F or higher. At least in some cases, lower carbon number components are reported for the stream, e.g. C5s at approximately 2% and benzene at up to 4%. The major components reported in the stream are typically 25% C9 compounds, 10 to 47% naphthalene, and 4 to 30% methylnaphthalenes.
6. (FO 6) Hydrotreated Flux Oil: This is a hydrotreated fuel-oil-like stream with a carbon number distribution predominantly C10 to hydrocarbons with a boiling point of 650°F or higher. The stream may be produced as distillation bottoms from a pyrolysis gasoline hydrotreator unit. The components in the stream are predominantly aromatics, olefins, and cyclic or dicyclic compounds. This stream differs from the other fuel oils described above in that its diolefin and vinyl aromatic contents are very low.
7. (FO 7) Biphenyl Concentrate: Biphenyl concentrate is a coproduct of the benzene hydrodealkylation unit that is isolated by distillation from the HDA reactor effluent. The carbon number distribution for the stream is C7 to C18, with the major component reported to be 65 to 95% biphenyl.

8. (FO 8) Combined Fuel Oil from Benzene Hydrodealkylation (HDA) and Pyrolysis Fuel Oils: Ethylene process operations that include both a pyrolysis gasoline distillation unit and a benzene hydrodealkylation unit may combine the fuel oil streams from these two units resulting in a single isolated product. Fuel oil is produced in the benzene HDA process by the HDA reactors and separated as a distillation bottoms product. The carbon number distribution for this combined fuel stream is C9 through hydrocarbons with a boiling point of 650°F or higher, although relatively low levels of lower carbon number hydrocarbons may be present, e.g. 0.2% benzene. The major components reported in the stream include approximately 11% C9 aromatics to naphthalene, 7.5 to 12% dicyclopentadiene, 8 to 12% naphthalene, 22% methylnaphthalenes, and 25 to 35% biphenyl.

1.2 Purity/Impurities/Additives

Additives are not typically added to the streams in the Fuel Oils Category prior to shipment.

1.3 Physico-Chemical Properties

The 8 streams in this category contain several different hydrocarbons (Table 2) that can vary in composition not only between manufacturers but also for an individual manufacturer, depending on feedstock type and operating conditions. The 5 constituents listed in Tables 3 and 4 comprise significant proportions of these streams, which is why they were selected to represent the potential range of select physico-chemical (PC) properties of these streams, specifically, melting point and water solubility. The remaining properties, boiling point, vapor pressure, and Log P_{ow}, will be characterized by the measured data for two of the streams presented in Table 5. These data can be used to adequately characterize the 5 PC endpoints of substances in this category for the HPV Program.

Table 3. Summary of Calculated Physico-Chemical Properties for Selected Chemicals Contained by Streams in the Fuel Oils Category

Chemical	Melting Point (°C)	Water Solubility (mg/L @25°C)
Indene	24.36	372.1
Dicyclopentadiene	-16.78	51.9
Naphthalene	5.01	183.8
Methylnaphthalene	22.15	54.6
1,1'-Biphenyl	25.07	44.7

Calculated values derived by the EPIWIN program (EPIWIN, 1999).

Table 4. Summary of Measured Physico-Chemical Properties for Selected Chemicals Contained by Streams in the Fuel Oils Category

Chemical	Melting Point (°C)	Water Solubility (mg/L @25°C)
Indene	na	na
Dicyclopentadiene	32.0	na
Naphthalene	80.2	142.1
Methylnaphthalene	34.4	41.4
1,1'-Biphenyl	69.0	29.0

Measured values from the EPIWIN experimental database (EPIWIN, 1999).
na not available

Table 5. Summary of Measured Physico-Chemical Properties for Two Streams Contained in the Fuel Oils Category

Stream (CAS RNs)	Boiling Point (°C @760 mmHg)	Vapor Pressure (hPa @ 25 °C)	Log P_{ow}
Pyrolysis C10+ Fuel Oil (CAS RNs 68513-69-9, 68921-67-5)	114 to 248	4.0	3.3 to 5.4
Heavy Pyrolysis Fuel Oil (CAS RNs 68513-69-9, 64741-62-4, 69013-21-4, 8002-05-9)	201 to 340	2.1	3.4 to 5.0

The following sections identify the values used to define PC endpoints for endpoints and streams other than the two streams in Table 5.

1.3.1 Melting Point (Range)

Based on calculated values (Table 4), the streams in this category can have a melting point range of -16.78 to 25.07 °C. Based on measured values, the streams in this category can have a melting point range of 32.0 to 80.2 °C. The measured data are considered the appropriate primary data set to characterize the melting point range of category members.

1.3.2 Boiling Point (Range)

Based on measured values for two streams (Table 5), the remaining streams in this category can have a boiling point range of 114 to 340 °C. These measured data are consistent with process knowledge for this category and are considered the appropriate primary data set to characterize the boiling point range of the remaining category members.

1.3.3 Vapor Pressure (Range)

Based on measured values for two streams (Table 5), the remaining streams in this category can have a vapor pressure range of 2.1 to 4.0 hPa at 25 °C. The measured data are consistent with process knowledge for this category and are considered the appropriate primary data set to characterize the vapor pressure range of the remaining category members.

1.3.4 Octanol-Water Partition Coefficient (Log Pow Range)

Based on measured values for two streams (Table 5), the remaining streams in this category can have a log P_{ow} range of 3.3 to 5.4. These measured data are considered the appropriate primary data set to characterize the log P_{ow} range of the remaining category members.

1.3.5 Water Solubility (Range)

Based on calculated values (Table 4), the streams in this category can have a water solubility range of 44.7 to 372.1 mg/L. Based on measured values, the streams in this category can have a water solubility range of 29.0 to 142.1 mg/L. The measured data are considered the appropriate primary data set to characterize the water solubility range of category members.

1.4 Category Justification

The Fuel Oils Category was developed by grouping select ethylene manufacturing streams that exhibit commonality from manufacturing process and compositional perspectives. The manufacturing relatedness of the category streams is described in Appendix I. Compositionally, category streams are composed predominantly of C7 to C13 hydrocarbons, which are predominantly cyclic olefins and aromatics (Table 2), but some can also contain smaller proportions of saturated hydrocarbons in this carbon number range. Each of the streams share a number of constituents at varying levels, with indene, dicyclopentadiene, naphthalene, methylnaphthalene, and 1,1'-biphenyl included among the predominant constituents. Selected members were included in this category because they were also expected to exhibit similar biological effects because of their largely comparable compositions.

The strategy to demonstrate that the members of this category could be considered together in order to assess their human and environmental health hazards and fate for purposes of the HPV Program was to:

- develop aquatic toxicity, biodegradation, and physicochemical data for two category streams, Heavy Pyrolysis Fuel Oil and Pyrolysis C10+ Fuel Oil, which between them contain a range of chemical constituents found in the remaining steams,
- develop additional fate information to characterize photodegradation, hydrolysis, and environmental partitioning and distribution,
- use existing analog data to add to the weight of evidence for this category, and
- use existing mammalian and aquatic toxicity data to characterize the human and environmental health endpoints.

After evaluating the human and environmental health effects and fate data, it was determined that the results for all endpoints other than biodegradation were sufficiently similar to consider the substances listed in Table 1 as a category. With regard to the two tested complex streams, the similar environmental testing results can be explained by the similarity in composition of these streams, which had been previously established. The differences in composition between these two streams did not result in widely differing or conflicting results. Consequently, data from the two tested complex streams provided needed information to conduct “read-across” to the untested complex streams. Also, data for select analog substances will be used as additional weight of evidence to support some endpoints for the category.

Although the biodegradation results for the category substances and the analog show a relatively wide range, the remaining environmental fate endpoints will be similar across the category because the physicochemical properties for the chemical constituents are similar.

2 EXPOSURE AND USE

The Category and Stream Production

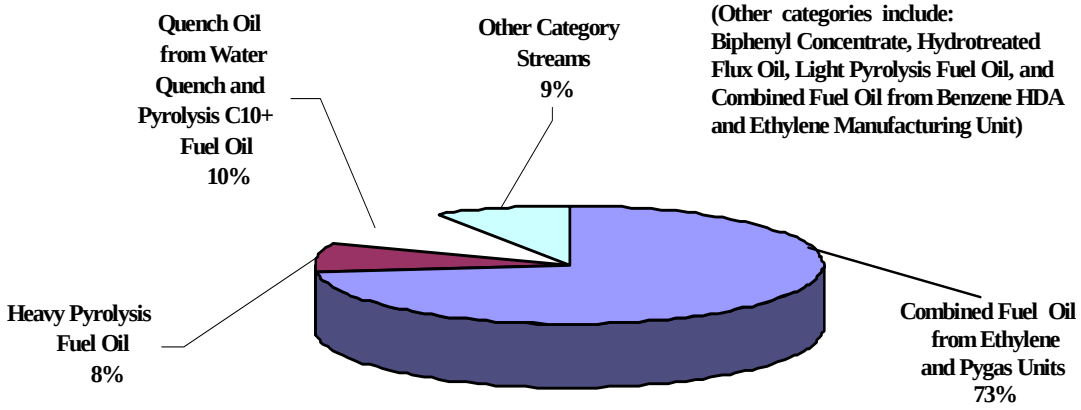
The Fuel Oils Category contains 13 CAS RNs (Table 1) that are associated with the following 8 process streams:

- Heavy Pyrolysis Fuel Oil (from the ethylene process unit)
- Quench Oil (from the ethylene process unit water quench system)
- Light Pyrolysis Fuel Oil (from the ethylene process unit)
- Pyrolysis C10+ Fuel Oil (from pyrolysis gasoline distillation)
- Combined Fuel Oil (E&P) (from the ethylene process and pyrolysis gasoline units)
- Hydrotreated Flux Oil
- Biphenyl Concentrate
- Combined Fuel Oil (B&P) (from benzene HDA and pyrolysis gasoline units)

The category streams are complex hydrocarbon mixtures, largely aromatics and cyclics, with variable compositions and a carbon range that is generally C10 and higher. Some of the streams also contain C7 to C9 hydrocarbons. The category streams are made up of the high molecular weight, high boiling hydrocarbons produced by the ethylene process. They are differentiated within the category by the specific location in the olefins processes where they are isolated. One of the streams is partially hydrogenated. The streams are isolated intermediates that are transferred under controlled conditions to a limited number of second parties that use the streams in a controlled way as an intermediate. The primary use of the streams is as blending streams for production of industrial or marine fuel oil. In limited cases, specific category streams are used to produce carbon black or used to produce heat transfer fluids.

Distribution of the 3.6 billion pounds/year[2] of category production among the category streams is shown in Figure 1. As indicated in the figure, the "Combined Fuel Oil from the Ethylene and Pyrolysis Gasoline Units" accounted for 73% of the category production in the reporting year.

Figure 1. Fuel Oils Category Production (1998 Data)



[2] 3.6 billion pounds per year is the approximate total annual commercial production of category streams reported by the sponsors of the Fuel Oils Category, based on their 1998 TSCA IUR (Inventory Update Rule).

Other industrial processes also produce some of the hydrocarbon compounds that make up the complex streams in this category. Potential exposures to these individual components from other manufacturing processes or from natural sources are considered to be out of scope for this assessment. This assessment is limited to potential exposures to the streams in the category. Some data are presented for specific components, which is intended to help clarify the potential for exposure to the category streams.

This screening level exposure assessment is based on information received from six of the seven sponsors of the category and upon other available information. The assessment does not include information on exposure potentials that may occur during use of the category streams, because that additional information was not available at the time of preparation of this report.

There are 13 CAS RNs that are used by the Olefins Industry to represent the 8 category streams (See appendix A). This assessment addresses the use of the CAS RNs for the Fuel Oils Category streams. Some of the CAS RNs in this category may be used by the Olefins Industry or others to represent substances that are not included in the Fuel Oils Category. These CAS RNs may be included in other HPV categories.

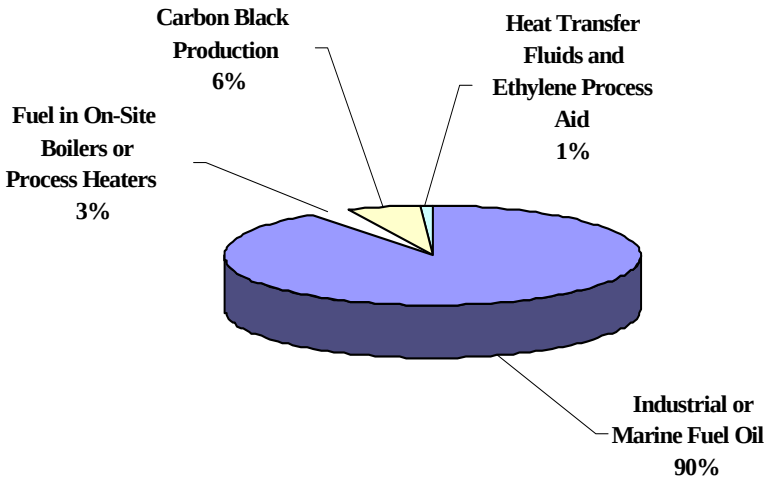
Storage and Transportation of Category Streams

When shipped between industrial sites, the category streams are transported in bulk by barge, pipeline, tank car or tank truck. The streams are typically inventoried in bulk storage tanks, either floating or fixed roof. Vents from loading and storage are typically controlled by a conservation vent or by routing to a control device, use of carbon canisters, or use of submerged fill for loading.

Use

Uses of the category streams are shown in Figure 2. There were no consumer uses reported for the category streams. The primary use of the category streams is for blending with other streams for the production of industrial or marine fuel oil. In some cases the streams are used on-site where they are produced as fuel in process heaters or boilers. Another use is for the production of carbon black, an intermediate used for example in the production of tires, rubber, inks, paints, and plastics. One other reported use is for the production of industrial heat transfer fluids. Figure 2 does not include use data for the following two category streams: Pyrolysis C10+ Fuel Oil (from Pyrolysis Gasoline distillation) and Combined Fuel Oil from Benzene Hydrodealkylation and the Ethylene Manufacturing Unit. Use information for these two streams was not available at the time this report was prepared. However, uses of these streams are expected to be similar to that of the other category streams.

Figure 2. Available Use Information for the Fuel Oils Category Streams (2001 Data) [3]



Route of Potential Exposure

The category streams are liquids with low vapor pressures at ambient conditions. Inhalation of vapors emitted from the streams and accidental dermal contact with the liquids are potential routes of exposure. The streams or components in the streams are slightly soluble in water and therefore groundwater contamination is possible in the event of spills or leaks from processing, during transportation, or from storage equipment.

Sources of Potential Exposure

Exposure to the category streams for workers in the Olefins Industry process units where the category streams are isolated is expected to be low because the processes and equipment are generally closed systems. In addition, emissions to air are expected to be low because of the low vapor pressure of the category streams and because the emission from storage and loading equipment are controlled by using floating roof storage tanks or by a conservation vent device or by routing vents from fixed roof storage tanks and loading equipment to control or recovery devices, including use of carbon canisters and submerged fill loading. For the industrial workers at these facilities, the most likely exposure potential occurs through inhalation of low-level concentrations in air of vapors that escape from the closed process, such as fugitive emissions from valve packing and from pump seals. Other potential for exposure may result during operations such as sampling, loading of bulk transportation vessels (tank cars, tanks trucks and barges), from emissions at floating roof or fixed roof storage tanks, or during infrequent opening of equipment for maintenance, and from emissions from control devices, such as flares.

Controls that Limit Exposure

The Occupational Safety and Health Administration (OSHA) established an 8-hour time-weighted average (8-hr TWA) Permissible Exposure Limit (PEL) for naphthalene of 10 ppm.[4] The

[3] The percentage uses of the category streams are based on data received from 6 of 7 category sponsors. Uses of 2 of the category streams are not included in Figure 2 because use information was not available at the time this report was written.

[4] http://www.osha.gov/pls/oshaweb/owadisp.show_document?p_table=STANDARDS&p_id=9991

ACGIH[5] adopted an 8-hr TWA threshold limit value (TLV) for naphthalene of 10 ppm and a short-term exposure limit (STEL) of 15 ppm.[6] Naphthalene is a component found in significant concentrations in the category streams.

Five of the seven sponsors of the category streams reported that they have programs that assess exposure to the category streams. Four of these included specific measurements for naphthalene or total hydrocarbons. Industrial hygiene programs for a specific production site are typically unique to the site and address the specific chemical exposure issues. Some of the components typically present in the category streams that have OSHA PELs or ACGIH TLVs are shown in Table 6.

Table 6. Components Typically Present in Streams of the Fuel Oils Category and that have OSHA PELs or ACGIH TLVs

Component	OSHA PEL	ACGIH TLV
Dicyclopentadiene	-	5
Biphenyl	0.2	0.2
Indene	-	10
Naphthalene	10	10

Among other reasons, the release of the category streams from process, storage and transportation equipment at industrial facilities is avoided because the streams are flammable liquids.

The category streams are mixtures of volatile organic compounds (VOC) and are therefore subject to USEPA and state environmental regulations that limit VOC emissions. The USEPA New Source Performance Standards (NSPS) of 40 CFR Part 60 may be applicable and limit emissions of VOC at new or modified Olefins process units where the streams in the category are produced. Subpart VV of NSPS limits emission from equipment leaks and subpart Kb limits emissions from VOC storage tanks. In addition, facilities that produce or use these streams and that are major sources may be subject to the National Emission Standards for Hazardous Air Pollutants for Source Categories: Generic Maximum Achievable Control Technology Standards, which includes ethylene manufacturing processes. State permits may also apply for specific facilities. These emissions control requirements reduce potential exposure to the category streams for the workers at facilities, the neighboring public, and the environment.

Ambient Concentration Data

Ambient air concentration data for the complex category streams was not available. Naphthalene is a component found in significant concentrations in the category streams. A NIOSH survey of worker exposures to polyaromatic hydrocarbons at a petroleum refinery in Tulsa, Oklahoma reported air concentrations of naphthalene as high as 10.2 ug/cu m in an area sample and 19.3 ug/cu m for a personal sample."[4]

Estimates of Potentially Exposed Workers

Naphthalene is a component found in significant concentrations in the category streams. "NIOSH (NOES Survey 1981 to 1983) has statistically estimated that 23,092 workers (2,171 of these are female) are potentially exposed to naphthalene in the US."[4] A number of limitations to this survey

5 Formerly known as the American Conference of Governmental Industrial Hygienists, now referred to only by the acronym.

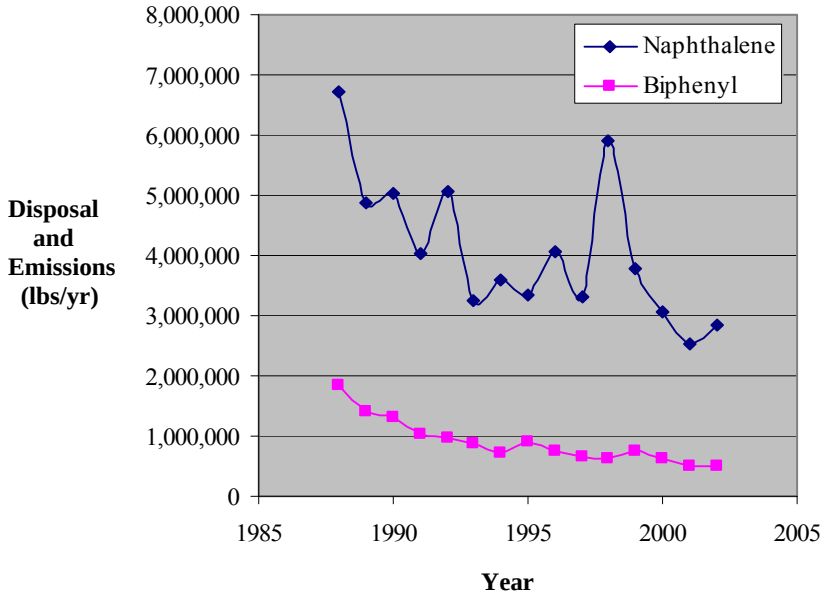
6 2003 TLVs and BEIs, Threshold Limit Values for Chemical Substances and Biological Exposures Indices, ACGIH, Cincinnati, OH, USA. 45240-1634.

have been identified over the years, and the estimates of the number of workers potentially exposed to various substances are generally thought to be high.

Category Emissions

Emissions quantities of the mixed streams are not available. Naphthalene and biphenyl are components expected to be found in significant concentrations in the category streams. Industrial emissions of naphthalene and biphenyl are reported to the EPA and made available to the public in the Toxics Release Inventory (TRI).[7] This inventory was established under the Emergency Planning and Community Right-to-Know Act of 1986 (EPCRA) and expanded by the Pollution Prevention Act of 1990. The TRI data indicate that reported emissions and waste of naphthalene have decreased by 57% from 6.7 million pounds in 1988 to 2.9 million pounds in 2002 (Figure 3). Biphenyl emissions and waste quantities decreased by 72% from a value of about 1.8 million pounds to about 0.5 million pounds in the same time period. However the relevance of individual component emissions values with regard to the category streams is uncertain, because the category streams likely account for only a portion of the total emissions of naphthalene and biphenyl.

Figure 3. TRI Naphthalene and Biphenyl Total Disposal and Emissions (lbs/year) for All Industries 1988 to 2002



Summary of Exposure Assessment

The Fuel Oils Category includes 8 commercial product streams from the Olefins Industry. The category streams are complex mixtures of variable composition and consist of the high molecular weight (generally carbon number 10 and higher) hydrocarbons produced by the olefins manufacturing processes. The primary use of the category streams is as blending streams for production of industrial or marine fuel oil. The streams are also used in limited cases for production of industrial heat transfer fluids or production of carbon black. The streams are sometimes used as fuel on site where they were produced. Thirteen CAS RNs are used to represent these streams. There are no known or expected consumer applications for these materials.

[7] EPA website for TRI: http://www.epa.gov/tri/

The category streams are transported for use to other industrial facilities in bulk by barge, pipeline, tank car, or tank truck.

Inhalation is a likely route of potential exposure although the volatility of the hydrocarbon components that make up the streams is low. Other possible exposure routes include dermal (from spills) and oral (from contaminated ground water), although these pathways are considered minor as compared to inhalation.

Occupational exposure is limited because production and use of these streams is generally in closed systems, and because of the low vapor pressure of the streams. Occupational exposure limits apply to some of the components in the category streams (naphthalene, biphenyl, dicyclopentadiene, and indene) and compliance with these limits reduces or prevents occupational exposure to these streams.

Environmental exposure is limited since emissions from production and use are limited and controlled by a number of volatile organic compound and hazardous air pollutant environmental regulations at both the federal and state level.

3 ENVIRONMENTAL FATE

3.1 Photodegradation

Environmental compartments of interest when considering the fate of constituents in Fuel Oil streams include surface water and the atmosphere, based on modelled data (see Section 3.3) that characterize their potential to partition to these compartments. The modelling results can be largely explained by the relatively high vapor pressure and water solubility of select constituents evaluated. In spite of their water solubility, wet deposition of category constituents is not likely to play a significant role in their atmospheric fate. Constituents of streams in this category have the potential to degrade at a significant rate in the atmosphere through indirect photolytic process mediated primarily by hydroxyl radicals (OH^-). In comparison, direct photolysis is not expected to contribute significantly to the degradative fate of these streams in the aqueous environment.

3.1.1 Direct Photodegradation

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982a). The reaction process is initiated when light energy at a specific wavelength elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non-excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982a). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982a). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light at wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977). Although the streams in this category are composed largely of unsaturated hydrocarbons, some can contain saturated hydrocarbons. Saturated hydrocarbons do not absorb light above 200 nm and therefore, those stream constituents have a low potential to photolyze. Characteristic absorbance maxima (λ_{max}) and associated molar absorptivities (ε) for four unsaturated hydrocarbons, which are examples of some constituents (Table 2) in category streams containing double bonds, are listed in Table 7 (Harris, 1982a). The constituents of streams in the Fuel Oils Category would have absorbance maxima and associated molar absorptivities (extinction coefficient) in the range of those chemicals in Table 7.

Table 7. Characteristic Absorbance Maxima (λ_{max}) and Associated Molar Absorptivities (ε) of Selected Unsaturated Hydrocarbons from Streams in the Fuel Oils Category

Hydrocarbon	λ below 290 nm		λ above 290 nm	
	λ_{max*}	ε	λ_{max*}	ε
1,3-Butadiene	217	20,900	-	-
Benzene	255	215	-	-
Naphthalene	221	100,000	311	250
	270	5,000	-	-
Biphenyl	246	20,000	-	-

* Values developed in organic solvents and regarded as approximate absorption maxima in aqueous solution.

Olefins with one double bond or cumulated double bonds, which constitute the majority of the chemicals in the Fuel Oils Category, do not absorb appreciable light energy above 290 nm. Streams in this category do not contain constituent molecules of significant concentration that will undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical constituents in this category from the environment.

3.1.2 Indirect Photodegradation

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH^-) radicals (Atkinson, 1988; Atkinson, 1989). The rate at which an organic compound reacts with OH^- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon an average atmospheric concentration of hydroxyl radicals.

Since the reactions necessary for this degradative process only take place in the presence of sunlight, the atmospheric half-lives are normalized to a 12-hour day. The five chemicals selected to represent the atmospheric half-life range of streams in this category are hydrocarbons that are predominant among the category CAS RNs (Table 8).

Atmospheric oxidation via hydroxyl radical attack can be a significant route of degradation for streams in this category. Based on calculated values, chemicals in streams from this category can

have an atmospheric half-life range of 1.1 to 53.0 hours as a result of indirect photolysis by hydroxyl radical attack.

Table 8. Hydroxyl Radical Photodegradation Half-life of Selected Chemicals from Streams in the Fuel Oils Category

Chemical	Calculated Half-life* (hrs)	OH^- Rate Constant (cm^3/molecule-sec)
Indene	53.0	2.4 E-12
Dicyclopentadiene	1.1	119.2 E-12
Naphthalene	5.9	21.6 E-12
Methylnaphthalene	2.3	56.5 E-12
1,1'-Biphenyl	18.9	6.8 E-12

* Atmospheric half-life values are based on a 12-hr day and an OH^- concentration of 1.5E6, which is the default concentration used by the model.

3.2 Stability in Water (Hydrolysis)

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H_2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982b). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule. The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond.

The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Under strongly acidic conditions the carbon-carbon double bond found in alkenes, such as those in the Fuel Oils Category, will react with water by an addition reaction mechanism (Gould, 1959). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (Harris, 1982b). This reaction differs from other reactions with water such as hydration of carbonyls that can lead to the formation of an alcohol beginning with the transfer of a proton from the water to an alkene. However, water by itself is too weak an acid to transfer a proton in the absence of a strong acid, which could effect such an acid catalyzed electrophilic addition.

Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985). The chemicals in this category are primarily aromatics and olefins (alkenes) that contain at least one double bond. However, streams in this category can contain smaller amounts of saturated hydrocarbons (alkanes). These groups of chemicals contain only carbon and hydrogen. As such, their molecular structures are not subject to the hydrolytic mechanisms described above (Harris, 1982b) under conditions typically found within the environment. Therefore, this fate process will not contribute to the degradative loss of chemical constituents in this category from the environment.

3.3 Distribution in the Environment

Fugacity-based multimedia modeling provides basic information on the relative distribution of a chemical between selected environmental compartments, which can include air, soil, water, sediment, suspended sediment, and biota. A widely used fugacity model, the EQC (Equilibrium

Criterion) Level I model (Mackay *et al.*, 1996; Mackay, 1998) calculates chemical distribution between these compartments based on the input of basic physicochemical parameters including molecular weight, water solubility, log P_{ow}, and melting point.

Results of the EQC Level I model (Table 7) for selected chemical constituents of streams from this category suggest that they will partition largely between the air, water, and soil compartments, with a negligible amount partitioning to sediment. These results can be largely explained by the relatively high vapor pressure and water solubility of select constituents evaluated. Distribution of these chemicals to each remaining compartment (suspended sediment and biota) is calculated as less than 0.1%.

The five chemicals selected to characterize the transport/distribution of category members range in carbon number between C9 to C12 and are predominant across the streams in this category. Physical property data (Tables 3 and 4) used in the model are from the EPIWIN (1999) database.

Table 9. Environmental Distribution as Calculated by the EQC Level I Fugacity Model for Selected Chemicals from Streams in the Fuel Oils Category

Chemical	Distribution Per Environmental Compartment (%)					
	Air	Water	Soil	Sediment	Suspended Sediment	Biota
Indene*	47.61	31.05	20.86	0.46	<0.01	<0.01
Dicyclopentadiene**	98.55	0.63	0.80	0.02	<0.01	<0.01
Naphthalene**	42.27	20.56	36.33	0.81	<0.01	<0.01
Methylnaphthalene**	98.53	0.19	1.25	0.03	<0.01	<0.01
1,1'-Biphenyl**	11.68	9.15	77.40	1.72	<0.02	<0.02

* Distribution values determined using calculated input data from the EPIWIN program
** Distribution values determined using input data from the EPIWIN program experimental database.

3.4 Biodegradation

Biodegradation is the use of a chemical by microorganisms as a source of energy and carbon. The parent chemical is broken down to simpler, smaller chemicals, which can eventually be converted to inorganic forms such as carbon dioxide, nitrate, sulfate, and water, depending on the composition of the parent chemical.

The microbial metabolism of aliphatic alkenes can be initiated by attack at the double bond (Watkinson and Morgan, 1990). Four degradative processes have been identified:

- Oxygenase attack upon a terminal methyl group to the corresponding alcohol, aldehyde, and acid
- Subterminal carbon oxygenase attack to the corresponding alcohol and ketone
- Oxidation across the double bond to the corresponding epoxide
- Oxidation across the double bond to the corresponding diol

Biodegradation test results are available for two complex category streams (EMBSI, 2004a, 2004b) and an additional complex stream that contains a significant proportion of 1,1'-biphenyl (Douglas, 1993), which is not a member of the category, but used as an analog to support the category. The standard test guidelines applied were the OECD (Organization for Economic Co-operation and Development) 301F, Manometric Respirometry Biodegradation Test and OECD 301D, Closed

Bottle Biodegradation Test. Both test methods use closed systems, which is necessary when evaluating volatile substances. The 28-day results for the two of the three complex streams, Heavy Pyrolysis Fuel Oil and Pyrolysis C10+ Fuel Oil, were 29 and 7% respectively (Table 10). The 28 day result for Biphenyl Feedstock was 57%.

Table 10. Summary of Biodegradation Data for Two Complex Streams in the Fuel Oils Category

CAS RN and Substance Name	Biodegradation (%)					
	Day 7	Day 8	Day 12	Day 14	Day 21	Day 28
Heavy Pyrolysis Fuel Oil 68513-69-9, 64741-62-4, 69013-21-4, 8002-05-9 (EMBSI, 2004a)	9.4	10.6	19.4	24.5	27.0	29.0
Pyrolysis C10+ Fuel Oil 68513-69-9, 68921-67-5 (EMBSI, 2004b)	1.0	1.6	1.0	1.3	3.5	7.3

EMBSI, ExxonMobil Biomedical Sciences, Inc.

These data can characterize the potential biodegradability of untested streams in this category. The data suggest that the untested streams in this category may biodegrade at a slow to moderate rate during a 28-day test period. Additionally, the analog substance showed no inhibitory affect on the normal degradative activity of the microbial inoculum used to evaluate its biodegradability (Douglas, 1993).

4 HUMAN HEALTH HAZARDS

4.1 Effects on Human Health

4.1.1 Acute Toxicity

Studies in Animals

A summary of the available oral, dermal, and inhalation acute toxicity studies is provided in Table 11. An acute oral toxicity with Light Pyrolysis Fuel Oil was conducted in Fischer 344 rats at doses of 0, 2.5, 2.75, 3.0, and 3.25 g/kg (Rausina, 1984). Observations for mortality and moribundity were performed daily until sacrifice on day 15. The most frequently observed clinical signs were nasal and ocular discharges, lethargy, and soft stools. No effects were seen on body weight. Gross necropsies revealed no adverse findings. Females were somewhat more susceptible than males and the LD50 for combined sexes (95% confidence interval) was determined to be 2.89 g/kg (2.63-3.28).

An acute dermal toxicity test with Biphenyl Feedstock was conducted on male and female New Zealand White rabbits at a limit dose of 2 g/kg (Rausina, 1983). One treated female died on day 1 of the study but no clinical signs were observed before the death. The other 9 rabbits appeared normal throughout the 14-day observation period. Body weights remained stable during the study and gross

necropsies on all rabbits showed no findings attributable to test article administration. The LD50 was not reached at a single dermal dose of 2 g/kg.

An acute inhalation toxicity test with Biphenyl Feedstock was conducted on male and female Fischer 344 rats at a limit dose of 3 g/m^3, which was the maximum attainable concentration (Gordon, 1982). No deaths occurred from the single 4-hour exposure. Immediately after exposure, all rats were covered with crystalline test article. Nearly every rat had dry red material around the nose and mouth, perianal soiling, clear ocular discharge, porphyrin around the eyes, and discolored fur. Two males and one female showed labored respiration. These symptoms subsided during the observation period and at sacrifice, only discolored fur was seen. Body weight was unchanged and no test article related lesions were detected at necropsy.

Table 11. Summary of Acute Toxicity Data for the Fuel Oils Category[1]

CAS RN and Substance Name	Oral (Rat)	Dermal (Rabbit)	Inhalation (Rat, aerosol)
Aromatic Pyrolysis Oil (FO1) 64742-90-1	>5 g/kg (Limit)	-	>3.7 g/m^3
Light Pyrolysis Fuel Oil (FO3) 68527-18-4	2.89 g/kg (2.63 - 3.28)	-	>4.95 g/m^3
Heavy Pyrolysis Hydrocarbons[2] (Rerun Tower Bottoms)	14.5 g/kg (11.5 - 18.3)	>5 g/kg (Limit)	~6.0 g/m^3 >6.6 g/m^3 (140˚ Vapor)
Biphenyl Feedstock[2] 68989-41-3	3.7 g/kg (3.3 - 4.2)	>2 g/kg (Limit)	>3 g/m^3
EDS Experimental Fuel Oil[2]	>5 g/kg (Limit)	>3.16 g/kg (Limit)	-

[1] Studies acknowledged in the Reference section.
[2] Materials of similar composition to category streams used as read-across data.
Note: The CAS RNs and stream names in represent the nomenclature reported for the test substances at the time of the study. The sponsors of streams in this category use other nomenclature, as indicated in Table 1 of this report.

Conclusion

Acute toxicity of the Fuel Oils Category can be adequately assessed with the available data. Tested streams in this category all exhibit minimal acute toxicity by the oral (>2.5 g/kg), dermal (>2 g/kg), and inhalation (>3 g/m^3) routes of exposure.

4.1.2 Repeated Dose Toxicity

Studies in Animals

Repeated dose toxicity studies have been conducted on a variety of the Fuel Oils Category streams (Table 12). The studies range from 8 to 90 days in duration and have been conducted in rats (oral, dermal, and inhalation) and rabbit (dermal).

Oral

In a ninety-day oral toxicity study, groups of 18 male and 18 female Sprague-Dawley rats were exposed to 0, 0.02, 0.1, or 0.5 g/kg/day EDS Experimental Fuel Oil diluted in highly refined white oil (McKee *et al.*, 1987). Exposures were conducted once daily, five days per week, for 13 weeks.

Administration at 0.5 g/kg/day for 13 weeks induced slight systemic toxicity including reduced body weight gain, elevated liver weight, reduced hematology values, and elevated cholesterol. No treatment related mortality or significant differences in food consumption or clinical signs were observed, except for urogenital staining in high dose animals. Body weight gain was significantly reduced in high dose males; weight gain in high dose females and all other treated animals was similar to controls. No apparent abnormalities in gross examination of visceral organs and no effects on organ weight of males in any group were observed. Absolute liver weight was elevated and brain weight was reduced in high dose females ($p<0.05$); brain weight was not significantly different from controls as a fraction of body weight. No treatment related microscopic changes in tissues from either sex in the high dose group were observed compared to controls. There were no gross lesions or masses. Erythrocyte counts, hemoglobin and hematocrit were significantly reduced in high dose females; hemoglobin was reduced in high dose males. Dose related changes in serum cholesterol (elevated) and SGOT (currently referenced in the scientific literature as aspartate aminotransferase or AST) levels (reduced) in high dose animals but fell within normal historical range of biological values. Other clinical chemistry parameters were not significantly different from concurrent vehicle control values. A no observed adverse effect level (NOAEL) of 0.1 g/kg/day, based on hematology and clinical chemistry effects at 0.5 g/kg/day, was identified.

Dermal - Rabbit

EDS Experimental Fuel Oil (50 and 200 mg/kg) was diluted in Primol 185, and administered at 2 ml/kg/day for 5 consecutive days per week during a 28-day dermal toxicity study (McKee *et al*., 1985). Test material was applied to unabraded skin in an area of approximate 200 cm^2 on the dorsal surface between the shoulders and lumber region.

No mortality occurred during the study. The test substance elicited dermal irritation as well as systemic effects that might have been related to weight loss or stress. At the site of application, desquamation, blanching, atonia, and fissuring were observed in the high dose group. The low dose group and controls showed only a low incidence of desquamation. There was a dose-related decrease in mean group body weight of both males and females that became more pronounced over time; however, significance was reached only in the high dose females. Food consumption was also reduced but not to levels of statistical significance.

All dosed rabbits showed statistically significant, dose-related increases in liver weight and liver to body weight ratio. Hepatic alterations were manifested as liver enlargement, gross observations of liver abnormalities, and microscopic findings of diffuse hepatocytomegaly, cytoplasmic degeneration and hepatocellular vacuolization. Blood cholesterol levels were significantly elevated in a dose related manner in both sexes; other clinical chemistry values were within normal ranges. Kidney weight and kidney to body weight ratio was elevated in both sexes, in a dose responsive manner, but no histopathological abnormalities were observed. Thymic atrophy was observed in high dose rabbits, but not in the low dose group. No other microscopic abnormalities were observed. A LOAEL of 50 mg/kg/day based on body weight reduction, liver weight increase, and serum cholesterol increase was estimated.

Dermal - Rat

Three separate repeat dose dermal toxicity studies were conducted on Aromatic Pyrolysis Oil, Light Pyrolysis Fuel Oil, and Biphenyl Feedstock in Fisher 344 rats exposed to 0, 1, or 2 g/kg/day.

Aromatic Pyrolysis Oil - A repeated dose dermal toxicity study was conducted for 6 h per day, for 9 days over a 14-day period (Zellers, 1983). No deaths or moribund rats were observed. Food consumption was decreased in all test article dosed rats; in males the decrease was dose related. In both males and females body weight was reduced in a dose-related manner. Dermal effects were difficult to evaluate because of the black/tarry test material; however, in the high dose group, after a weekend without dosing, erythema was moderate to severe with fissuring and skin peeling. Skin

effects consisted of moderate to marked acanthosis and hyperplasia of the epithelium, and hyperkeratosis. No other test article related histopathologic lesions were found. There were no statistically significant changes in clinical chemistry and hematology parameters. Elevated liver weight was observed in all treated groups. Aromatic pyrolysis oil caused depression of body weight gain associated with decreased food consumption. At 2 g/kg/day, all rats showed moderate to severe erythema (Draize score 3-4). Fissures and peeling skin were seen at 2 g/kg/day but not at 1 g/kg/day. A LOAEL of 1 g/kg/day was determined based on depression of body weight gain.

Light Pyrolysis Fuel Oil - A repeated dose dermal toxicity study was conducted for 6 h per day, for 5 days over an 8-day period (Rausina, 1985). No mortality or morbidity was observed and there were no test article related clinical signs. By day 5, males and females in both dose groups had well defined erythema, with some resolution and eschar formation by day 8. Slight edema was seen in the high dose males and females that resolved by day 8. A significant decrease in body weight was noted in high dose males. Mean body weight was decreased in males in the 2.0 g/kg/day group. Skin irritation occurred that partially resolved after the two-day recovery period with severe erythema/eschar formation in the high dose group. A LOAEL of 1 g/kg/day was determined based on skin irritation.

Biphenyl Feedstock - A repeated dose dermal toxicity study was conducted for 6 h per day, for 9 days over a 12-day period (Rausina, 1983). No mortality or moribundity was observed during the study. Body weights were reduced but the effect was statistically significant only in females. No dermal reactions or test article related clinical signs were observed. There were no biologically significant test article related changes in the hematology or clinical chemistry parameters. However, sera of test article-treated rats were more yellow than that of controls. There was an increase in absolute weight of kidneys of males and females in the test article groups that was significant only for female left kidney. There were no gross pathological changes in skin at the site of application. There were no histopathological lesions that could be attributable to test article exposure. Dosing with the test article did not produce overt toxicological effects but there were decreases in terminal body weight and increases in specific organ weight that appeared to be treatment related. A LOAEL of 1 g/kg/day was determined based on reduction in body weight.

Inhalation

Aromatic Pyrolysis Oil - A repeat dose inhalation toxicity study was conducted in Fisher 344 rats exposed to 0, 0.54, or 2.00 g/m^3 for 6 h per day, for 9 days over a 12-day period (Gordon, 1983). No mortality or morbidity was observed. Males and females showed dose-related decreases in body weight and increases in clinical symptoms (hair loss, nasal discharge, discharge from eyes, eyes closed and perianal soiling). The organ weights of the high dose male and female livers, the high dose female lungs and the low dose female livers were significantly increased relative to control animal values. The spleen weights of the high dose male and female rats were significantly decreased. A decrease was observed in the high dose male heart weights compared to control male data. Clinical pathology values were unremarkable. Treated rats, showed yellow discoloration of the lungs grossly and hyperplasia of the pulmonary alveolar macrophages microscopically. At the high dose, one female showed arching of the back. Skin irritation was observed at both dose levels, which resolved after the 2 days recovery period in the 0.54 g/m^3 dose group. Frequency and severity of effects were related to exposure level. A LOAEL of 0.54 g/m^3 was determined.

Light Pyrolysis Fuel Oil - A repeat dose inhalation toxicity study was conducted in Fisher 344 rats exposed to 0, 0.51, 1.26, or 2.54 g/m^3 for 6 h per day, 5 d per week, for a 4 week period (Rausina, 1985). After four exposures to 2.54 g/m^3, 75% of the rats were dead or moribund. After the last exposure, two females at the 1.25 g/ m^3 level were sacrificed moribund. No other mortality was observed. The most frequent clinical signs in all dose groups were ocular porphyrin and discharge, closing of the eyes and nasal discharge; the highest incidence was in the 2.54 g/m^3 group. Significant decreases in body weight were present in all test article exposed groups, and, with the

exception of the spleen, were associated with consistent increases in organ to body weight ratios. Both clinical signs and body weight changes were correlated with dose. Total white blood cell and platelet counts were elevated at 1.26 g/m^3, and occasionally at 0.51 g/m^3; decreased mean corpuscular hemoglobin was seen in females of both these dose groups, and in males at 0.51 g/m^3. White cell increases were attributed to increased numbers of segmented neutrophils. Blood glucose levels were increased in males and females at 2.54 g/m^3 and in males at 1.26 g/m^3. Gross pathological effects included alopecia, perianal soiling, abnormal coloration of liver, lack of body fat. There was a variety of histopathological findings with the most severe being necrosis of cortical thymus lymphocytes especially in the high dose females. Atrophy of the thymic cortex was seen in 1.26 and 2.54 g/ m^3 males and females. Atrophy of splenic lymphoid tissue, especially in high dose females, lymphoid hyperplasia in lungs, and hypoplasia of bone marrow accompanied changes in the thymus. Hyaline droplets were observed in male kidneys in the 1.26 and 2.54 g/ m^3 groups. Generalized vascular congestion was seen in both sexes in the 1.26 and 2.54 g/ m^3 groups, which was particularly prominent in bone marrow, kidney, adrenal, lung and thymus. A LOAEL of 0.51 g/ m^3 was determined based on decreased body weight, hematocrit, hemoglobin and blood glucose.

Biphenyl Feedstock - A repeat dose inhalation toxicity study was conducted in Fisher 344 rats exposed to 0, 1.07, or 3.04 g/m^3 for 6 h per day, for 9 days over a 12-day period (Gordon, 1983).

There were no test article-related deaths during the study. Males and females showed dose related weight loss. Most of the dosed rats showed perianal soiling, excessive ocular porphyrin, dry red matter around mouth and nose, and crystalline test article on fur. There were no biologically significant effects of the test article on clinical chemistry or hematology parameters. However, there was a dose-related yellowing of blood sera. There were significant increases in absolute liver and kidney weight of high dose females, and decreases in spleen weight of high dose males. There were many significant increases in organ/body weight ratios owing to decreased weight gain in treated rats. There were no microscopic changes in male or female organs/tissues attributable to exposure. The only effect that was noted at gross necropsy was skin discoloration in treated rats. A LOAEL of 1.07g/m^3 based on body weight loss was determined.

Pyrolysis C10+ Fuel Oil (Rerun Tower Bottoms) - A repeat dose inhalation toxicity study was conducted in Fisher 344 rats exposed to 0, 0.15, 0.74, or 5.1 g/m^3 for 6 h per day, for 10 days over a 12-day period (Rose *et al*., 1984). No deaths occurred during the study. Clinical signs observed in the 5.1 g/m^3 group were abnormal body posture and closing or partial closing of eyes consistent with exposure to an irritant atmosphere. Following exposure, some high dose animals exhibited lethargy, red/brown staining around head or snout, urine staining, salivation, occasional ataxia and lacrimation, peripheral vasodilation, and hair loss. Increased urination was noted in the high dose for both sexes. At 5.1 g/m^3, males failed to gain weight resulting in a significant difference compared to controls while females gained less than controls but the effect was not statistically significant. Overall, food consumption was significantly lower in the high dose group and both sexes consumed significantly more water. High dose males exhibited significantly higher values for packed cell volume, hemoglobin, and red blood cell count. Lower dose groups showed few clinical signs. Body weight and weight gain was similar to controls in the 0.15 and 0.74 g/m^3 groups.

The high dose males had significantly higher protein, albumin, and serum glutamic-pyruvic transaminase (SGPT – currently referenced in the scientific literature as alanine aminotransferase or ALT) levels and significantly lower alkaline phosphatase level than controls. In females, the albumin/globulin (A/G) ratio and SGPT levels were higher than controls. The A/G ratio in 0.74 g/m^3 females was also higher than controls. Urea nitrogen levels in females at all dose levels were significantly lower than controls. At necropsy, increased incidence of alopecia and incidence of hemorrhagic areas in the mucosa of stomachs in 5.1 g/m^3 female rats was observed macroscopically. Liver, kidney and adrenal weight tended to be higher than controls for most groups in a dose-related fashion; spleen and thymus weight in 0.74 g/m^3 and 5.1 g/m^3 groups tended to be less than controls. Differences were significant for males at all dose levels for kidney weight,

at 0.74 and 5.1 g/m^3 for liver (increase) and spleen (decrease), and at 5.1 g/m^3 for adrenal (increase) and thymus (decrease). In females, changes were statistically significant only at 5.1 g/m^3. Microscopic pathology results in the high dose group showed enlargement of centrilobular hepatocytes in liver, decreased cellularity of red pulp in spleen, minimal involution of thymus, minimal increase in fine vacuolization of zona fasciculata, and minimal increase in cortical width in adrenals. Male rats from all dose groups had eosinophilic intracytoplasmic inclusions in renal cortical tubules in the kidney. This effect is now correlated with characteristic hydrocarbon-induced nephropathy seen in male rats. A LOAEL of 0.15 g/m^3 was determined based on changes in kidney weight and pathology (males) and decreased urea nitrogen levels (females).

Table 12. Summary of Repeated Dose Toxicity Data for the Fuel Oils Category

CAS RN and Substance Name	Oral	Dermal	Inhalation (aerosol)
Aromatic Pyrolysis Fuel Oil * 64742-90-1	-	LOEL 1 g/kg/day (2 wk; rat)	LOEL 0.54 g/m^3 (12 d; rat)
Light Pyrolysis Fuel Oil 68527-18-4	-	LOEL 1 g/kg/day (8 d; rat)	LOEL 0.51 g/m^3 (28 d; rat)
Heavy Pyrolysis Hydrocarbons (Rerun Tower Bottoms)*	-	-	LOEL 0.15 g/m^3 (12 d; rat)
Biphenyl Feedstock* 68989-41-3	-	LOEL 1 g/kg/day (12 d; rat)	LOEL 1.07 g/m^3 (12 d; rat)
EDS Experimental Fuel Oil*	NOAEL 0.1 g/kg/day (90 d; rat)	LOAEL 50 mg/kg/day (28 d; rabbit)	-

* Materials of similar composition to streams in this category used as read-across data.

Conclusion

Data are available to adequately characterize the repeated dose toxicity of the Fuel Oils Category. Oral, dermal and inhalation studies have been conducted on several representative streams that comprise this category. The most consistent observations among the studies were decreased body weight (often associated with reduced food consumption) and alterations in clinical chemistry and hematology parameters. Dermal irritation and ocular discharge were also often noted. For EDS Experimental Fuel Oil, an oral no observed adverse effect level (NOAEL) of 0.1 g/kg/day was identified based on hematology and clinical chemistry effects at 0.5 g/kg/day. A dermal LOAEL of 50 mg/kg/day based on body weight reduction, liver weight increase, and serum cholesterol increase was estimated for this material. Inhalation toxicity is adequately represented by Heavy Pyrolysis Fuel Oil (Rerun Tower Bottoms) in which a LOAEL of 0.15 g/m^3 was determined based on changes in kidney weight and pathology (males) and decreased urea nitrogen levels (females).

4.1.3 Mutagenicity

Genetic toxicity has been evaluated in several of the Fuel Oils Category streams in both *in vitro* and *in vivo* assays (Table 13).

In vitro

Unscheduled DNA Synthesis:

Primary rat hepatocytes were treated with Aromatic Pyrolysis Oil at concentrations of 0.5, 2.0, 10, and 60 µg/ml to evaluate genetic damage by induction of unscheduled DNA synthesis (Brecher and Goode, 1984). Aromatic Pyrolysis Oil induced toxicity in primary hepatocytes beginning at 4µg/ml following 18 to 20 hours exposure. Viability continued to decrease in a generally dose related manner to the maximum dose of 1024 µg/mL. Unscheduled DNA Synthesis (UDS) occurred in a dose-related manner, increasing from 117 net nuclear grains at 2 µg/ml to 218 grains at 60 µg/ml compared to a vehicle control net count of 0.63 and positive control of 363 net nuclear grains. Aromatic Pyrolysis Oil induced a dose related increase in UDS in cultured rat hepatocytes. Aromatic Pyrolysis Oil caused DNA damage and repair in this assay.

Concentrations of 8, 16, 32, 64, 128, 256, 512, and 1024 µg/ml of Light Pyrolysis Fuel Oil were added to cultures of primary rat hepatocytes to evaluate induction of unscheduled DNA synthesis (Brecher, 1984). Light Pyrolysis Fuel Oil induced significant toxicity (at ≥ 64 µg/ml) following 18 hours exposure. Percentage of cells in repair increased from the vehicle control value of 2.7% to 43.3% at 8 µg/ml to 96% at 32 µg/ml. Light Pyrolysis Fuel Oil caused dose-related UDS at all non-toxic levels. Positive and negative controls gave expected responses. Light Pyrolysis Fuel oil caused DNA damage and repair under the conditions of this assay.

Assessment of genetic damage and repair was evaluated by measuring unscheduled DNA synthesis in primary rat hepatocyte cultures treated with 0, 5, 20, 50, or 100 µg/ml Biphenyl Feedstock (Brecher and Goode, 1984). A range finding study was conducted at concentrations ranging from 4 to 2048 µg/ml to evaluate cytotoxicity. Biphenyl Feedstock induced toxicity in the 50 and 100 µg/ml dose groups (doses of 5, 20, 50, 100 µg/ml). Toxicity in the UDS assay occurred resulting in fewer than 150 viable cells available for counting in each of these groups. Despite this toxicity, Biphenyl Feedstock induced a positive, dose-related response for UDS at all doses evaluated, indicative of DNA damage and excision repair in this assay.

Chinese Hamster Ovary / Hypoxanthine-Guanine Phosphoribosyl Transferase:

Chinese Hamster Ovary cells were treated with Aromatic Pyrolysis Oil at concentrations of 32, 64, 96, 128, 175, and 256 µg/ml in the absence of S9, and 128, 175, 256, 375, 512, and 750 µg/ml in the presence of S9 (Papciak and Goode, 1984). A second experiment was conducted at concentrations of 500, 600, and 750 µg/ml to more adequately describe the dose response curve. Aromatic Pyrolysis Oil induced cell toxicity beginning at 32 µg/ml +S9 and at 256 µg/ml –S9. In the mutagenicity test, reduced cell count was seen at all dose levels ± S9. A significant increase in mutant frequency was observed at 750 µg/ml (+S9). No mutagenic effects were observed in nonactivated (-S9) cultures. In a repeat trial of the activated portion of the assay, APO induced a significant increase in mutant frequency at 500 µg/ml, while higher doses of 600 and 750 µg/ml were toxic. A linear dose response was observed over the clonable dose range. Positive control compounds demonstrated appropriate responses. Aromatic Pyrolysis Oil induced gene point mutations in the presence of rat liver metabolic activation under conditions of this assay.

Induction of mutations at the hypoxanthine-guanine phosphoribosyl transferase locus was evaluated in Chinese Hamster Ovary Cells treated with 0, 25, 32, 50, 64, and 128 µg/ml Light Pyrolysis Fuel Oil in the presence and absence of S9 (Papciak, 1984). Cytotoxicity was evaluated at the above concentrations of 8 and 16 µg/ml as well. Light Pyrolysis Fuel Oil induced cell toxicity at all dose levels with and without S9. No reduction in colony counts was observed in any non-activated dose groups with sufficient cells to clone (8, 16, 32 µg/ml). In S9 activated cultures, significant cloning toxicity occurred at 64 and 128 µg/ml. In the mutagenicity test, cell toxicity occurred at doses of 32 µg/ml and higher in –S9 cultures and at 16 µg/ml and higher doses in +S9 cultures. Cloning efficiency decreased in +S9 cultures at all doses. No significant increase in mutant colonies and no

dose-related response were observed in any culture –S9. A repeat activated test was performed at dose levels of 50 and 64 µg/ml. No significant increases in number of mutant colonies or a dose response were observed in the repeat assay. Positive control compounds demonstrated appropriate responses. Light Pyrolysis Fuel Oil did not induce a mutagenic response with or without metabolic activation and did not cause gene point mutations under the conditions of this assay.

Mutagenic activity of Biphenyl Feedstock was evaluated by treating Chinese Hamster Ovary cells with 0, 4, 8, 16, 21, 26, 32, and 64 µg/ml Biphenyl Feedstock in the presence and absence of S9 (Papciak and Goode, 1984). Cytotoxicity was assessed by treating cells with concentrations ranging from 4 to 2048 µg/ml. Biphenyl feedstock induced cytotoxic effects at concentrations of 32 µg/ml and higher –S9, and at 16 µg/ml and higher +S9. In the mutagenicity test, cell count toxicity was observed beginning at 8 µg/ml ±S9; cytotoxicity in colony counts occurred at 16 µg/ml and higher ±S9. Absolute survival was significantly decreased only in +S9 cultures at concentrations of 26 µg/ml and higher. There was no statistically significant increase in mutant frequency for any dose level of biphenyl feedstock compared to controls ±S9 in this assay. Positive and negative controls demonstrated appropriate responses. Biphenyl feedstock did not induce a mutagenic response with or without metabolic activation in CHO/HGPRT cells at any dose level. Cytotoxic effects were observed in both activated and non-activated cultures, demonstrating interaction of the test material with the cell system. Biphenyl Feedstock did not induce a mutagenic response with or without metabolic activation and did not cause gene point mutations under the conditions of this assay.

Ames *Salmonella* Assay:

Mutagenicity of Heavy Pyrolysis Fuel Oil (Rerun Tower Bottoms) was evaluated in strains of Salmonella bacteria and Sacchromyces yeast treated with 0, 0.001, 0.01, 0.1 1, and 5 µl/plate in the presence and absence of rat liver S9 (Brusick, 1977). The test substance was toxic to strains TA1535, TA1537, TA98, and S. cerevisiae D4 at 5.0 µl/plate. The test material did not increase revertant frequency in any Salmonella strain without metabolic activation. In the presence of S9 metabolic activation, no increase in revertant frequency was seen in TA1535, TA1537, TA100, and D4 in the first assay. A repeat test with TA98 and TA100 was performed at 1.0 and 5.0 µl/plate because these strains exhibited a dose-related increase in revertant frequency. Repeat assay was considered negative. The D4 test was repeated at doses of 1.0 and 5.0 µl/plate due to slight increased revertant frequency at 1.0 µl/plate in the first test and toxicity at 5.0 µl/plate. No increase in revertants was observed at 1.0 µl and toxicity persisted at 5.0 µl in the repeat assay. Rerun Tower Bottoms did not demonstrate reproducible mutagenic activity and was not considered to be mutagenic under these test conditions.

Ames assays were conducted for EDS Experimental Fuel Oil in strains TA 100 and TA98 ±S9, the strains potentially most sensitive to detect activity of complex hydrocarbons (Mckee *et al*., 1995). These strains were treated with concentrations of 0; 0.1; 1.0; 10; 50; 100; 500; 1,000; and 10,000 µg/ml in the presence and absence of hamster or rat liver S9. Positive, dose related increases in revertant frequencies were observed only in TA98 +S9. Positive and negative controls performed appropriately. EDS Experimental Fuel Oil is considered mutagenic in this system.

Mouse Embryo Cell Transformation - BALB/3T3:

The ability of Aromatic Pyrolysis Oil to induce transformations in mouse embryo cells was evaluated at concentrations of 0, 8, 16, 32, 64, 128, and 256 µg/ml (Brecher and Goode, 1983). Aromatic Pyrolysis Fuel Oil induced toxicity in BALB/3T3 cells at concentrations of 128 µg/ml after two days exposure. Maximum toxicity occurred between 256-512 µg/ml and reached a plateau at 1024 µg/ml. APO induced transformed foci at 128 and 256 µg/ml with borderline positive, but inconsistent, responses at concentrations between 8-64 µg/ml. Aromatic Pyrolysis Oil induced cell transformations in BALB/3T3 cell under the conditions of this assay. Cytotoxicity and impairment of cloning efficiency were also observed at the two highest dose levels.

Mouse embryo cells were treated with 0, 20, 60, 90, and 110 µg/ml of Light Pyrolysis Fuel Oil and cultures were evaluated for transformations (Brecher, 1984). Cytotoxicity was assessed in a separate exposure with concentrations ranging from 8 to 5000 µg/ml. Light Pyrolysis Fuel Oil induced toxicity in BALB/3T3 cells beginning at 32 µg/ml. Viability dropped sharply at 128 µg/ml and was 100% toxic at higher concentrations. Toxicity was evident at 60 µg/ml. Positive and negative controls gave expected responses. LPFO did not induce transformed foci in excess of negative control cultures at any dose level.

Biphenyl Feedstock was administered to BALB/3T3 cells at concentrations of 0, 4, 8, 16, and 32 µg/ml (concentrations in a pilot study ranged from 4 to 2048 µg/ml) to assess transformation of these cells in culture (Brecher and Goode, 1983). Biphenyl feedstock induced toxicity in BALB/3T3 cells beginning at 16 µg/ml, inducing reduction to 20% viability between 32 to 64 µg/ml and 2.1% viability at 2048 µg/ml. In the transformation assay, a progressive increase in cytotoxicity occurred with increasing doses from 8 to 32 µg/ml reducing the relative cloning efficiency. At 32 µg/ml, the toxic response was comparable to that of the positive control. The positive control induced the expected response (10 foci) for transformation. The vehicle control had 1 focus, but the untreated medium control was slightly higher with 2 foci. The 8 µg/ml and 32 µg/ml biphenyl feedstock cultures each had 2 foci. The results from treated cultures were considered to be negative. Biphenyl feedstock did not induce significant transformation in BALB/3T3 cells under conditions of this assay.

Sister Chromatid Exchange:

The ability of Heavy Pyrolysis Oil to induce sister chromatid exchange was evaluated in human lymphocytes treated with concentrations of 0, 0.02, 0.04, 0.06, 0.08, and 0.1 µl/ml (Galloway, 1981). These concentrations were selected following a pilot assessment with concentrations ranging from 0 - 3.3 µl/ml. No metaphases were found at 3.3 µl/ml that could be scored. At 1.11 µl/ml, 50 metaphases could not be found due to cell cycle delay and a reduction in mitotic index. However, there was a statistically significant increase in SCE at 1.11 µl/ml and 0.33 µl/ml. In the definitive study, pronounced cell cycle delay occurred at 0.08 and 0.10 µl/ml. There were statistically significant increases in SCE/cell at 0.06, 0.08, and 0.10 µl/ml compared to DMSO negative control with some evidence of a dose response, however doubling of SCE incidence over DMSO controls was not reached. Positive control compound (EMS) induced ~ 33 SCE/cell in both assays. While the SCE increase was not large, it was apparently dose related and Rerun Tower Bottoms was considered to show a weakly positive response under conditions of this assay.

Syrian Hamster Embryo:

Primary cultures of freshly derived hamster embryo cells were treated with concentrations of 0; 0.1; 0.5; 1.0; 5.0; 10; 50; 100; 500; and 1,000 µg/ml of EDS Experimental Fuel Oil for evaluation of mutagenic activity leading to cell transformation (McKee *et al*., 1995). Morphological transformation was induced in SHE cells over a concentration range of 1 to 100 µg/ml. Toxicity was observed at higher concentrations. Positive and negative controls performed appropriately. EDS Experimental Fuel Oil is a genetic toxicant.

Table 13. Summary of *In Vitro* and *In Vivo* Genotoxicity Data for the Fuel Oils Category

CAS RN and Substance Name	*In Vitro*								*In Vivo*
	CHO[1]		UDS[2]	SHE[3]	SCE[4]	BALB/3T3[5]	Ames[6]		MN[7]
	+S9	-S9					+S9	-S9	
Aromatic Pyrolysis Oil	+	-	+			+			+
Light Pyrolysis Fuel Oil	-	-	+			-			-
Heavy Pyrolysis (Rerun Tower Bottoms)					+ (weak)		-	-	
Biphenyl Feedstock*	-	-	+			-			-
EDS Experimental Fuel Oil*				+			+	-	

1 Chinese Hamster Ovary
2 Unscheduled DNA Synthesis
3 Syrian Hamster Embryo
4 Sister Chromatid Exchange
5 Mouse Embryo Cell Transformation Assay
6 Ames Salmonella
7 Mammalian bone marrow erythrocyte micronucleus
* Materials of similar composition used as read-across data to support the category.

In vivo

Mammalian Bone Marrow Erythrocyte Micronucleus Assay:

Groups of male and female ICR Swiss mice were treated with 0, 1.25, 2.5, and 5.0 g/kg of Aromatic Pyrolysis Oil by gavage to evaluate the induction of micronucleated polychromatic erythrocytes in bone marrow (Khan and Goode, 1984). Three groups of mice were given APO by oral gavage daily for two days. One half of each treated group and vehicle control (5M, 5F) was killed on day 3 and the remainder on day 4. One group (15M, 15F), given 5.0 g/kg by gavage in a single dose for 1 day only, was killed on days 2, 3, 4 (5/sex/day). Males treated with 1.25 to 5.0 g/kg Aromatic Pyrolysis Oil showed significant dose related increases in micronucleated polychromatic erythrocytes (PCE). Females showed significant increases in micronucleated PCE only at 5.0 g/kg. All mice given one dose of 5.0 g/kg showed positive responses compared to negative controls. There were no significant changes in the ratio of PCE/NORM (normochromatic erythrocytes) compared to controls. A LOEL of 1.25 g/kg was determined for males and a NOEL of 2.5 g/kg was determined for females. Aromatic Pyrolysis Oil induced cytogenetic damage in this test system.

Induction of micronucleated polychromatic erythrocytes in bone marrow was evaluated male and female ICR Swiss mice treated with 0.25, 0.5, and 1.0 g/kg by gavage of Light Pyrolysis Fuel Oil (Khan, 1984). Three groups of mice were given Light Pyrolysis Fuel Oil by oral gavage daily for two days. One half of each treated group and vehicle control (5M, 5F) was killed on day 3 and the

remainder on day 4. One group (15M, 15F), given 1.0 g/kg by gavage in a single dose for 1 day only, was killed on days 2, 3, 4 (5/sex/day). One of ten males given 1.0 g/kg Light Pyrolysis Fuel Oil died by day 3. No other mortality or significant weight changes were observed. Surviving mice did not show any significant changes in micronucleus formation in PCE and no significant changes in the ratio of PCE/NORM (normochromatic erythrocytes) compared to vehicle controls. A NOEL of 1.0 g/kg was determined for the genetic endpoint and a NOEL of 0.5 g/kg was determined for the systemic endpoint. Under these test conditions Light Pyrolysis Fuel Oil did not induce cytogenetic damage.

Biphenyl Feedstock was administered to male and female ICR Swiss mice at dose levels of 0, 0.25, 0.5, and 1.0 g/kg to evaluate micronucleus formation (Khan, 1984). Three groups of mice were given Light Pyrolysis Fuel Oil by oral gavage daily for two days. One half of each treated group and the vehicle control (5M, 5F) was killed on day 3 and the remainder on day 4. One group (15M, 15F), given 1.0 g/kg by gavage in a single dose for 1 day only, was killed on days 2, 3, 4 (5/sex/day). No mortality occurred at any dose level and no effects on body weight were observed in either sex. Mice treated with Biphenyl Feedstock did not show any significant change in the frequency of micronucleus formation in PCE and no significant changes in the ratio of PCE/NORM (normochromatic erythrocytes) compared to vehicle controls. A NOEL (genetic and systemic) of 1.0 g/kg was determined. Under these test conditions Biphenyl Feedstock did not induce cytogenetic damage.

Conclusion

Adequate in vitro and in vivo rodent data are available to characterize the genotoxic potential of Fuel Oils Category streams. The results of a diverse array of mutagenicity, cell transformation, and clastogenicity assays indicate positive responses in some assays and negative responses in others. Light Pyrolysis Fuel Oil, Heavy Pyrolysis Oil and Biphenyl Feedstock demonstrated activity in assays for general genetic damage, unscheduled DNA synthesis and sister chromatid exchange, but were generally inactive in assays for mutagenicity (HGPRT and Ames assays), clastogenicity (micronucleus) and cell transformation. Aromatic Pyrolysis Oil was determined to be mutagenic and clastogenic, induced DNA synthesis (indication of repair) and produced transformation in culture cells. EDS Experimental Fuel Oil was mutagenic in the Ames assay and transformed Syrian hamster embryo cells in culture. Mutagenic activity required metabolic activation. Using Aromatic Pyrolysis Oil as a worst case surrogate for the Fuel Oils Category, it is concluded that these streams are potentially genotoxic.

4.1.4 Carcinogenicity

Studies in Animals

In vivo

Two carcinogenicity studies were conducted on Pyrolysis Fuel Oil (Weil and Condia, 1977). Groups of 40 C3H/HeJ mice (sex not specified) were exposed three times per week for 28 months by skin painting. Doses of neat test article, water or benzene were brushed on to the backs of mice, clipped free of hair. Doses were applied qualitatively, with each dose described as one "brushfull". At monthly intervals, papilloma or carcinoma indices were calculated. Median latent periods were determined and lesions were verified by histopathology.

Oil-quenched and water-quenched Pyrolysis Fuel Oil were both highly carcinogenic. The oil-quenched papilloma and carcinoma indices were 94.4 and 94.4, respectively, and the median papilloma and carcinoma latent periods were 10.3 and 12.1 months, respectively. The water-quenched papilloma and carcinoma indices were 100 and 97.2, respectively, and the median papilloma and carcinoma latent periods were 10.2 and 12.2 months, respectively. The malignant tumors were squamous cell carcinomas. No tumors were observed in either control group.

Conclusion

Pyrolysis Fuel Oil was carcinogenic in the mouse skin painting bioassay. Although the method used a qualitative procedure of skin painting rather than exact volume application, and the material was not analyzed, the results were unambiguous. The described process conditions and the benzo(a)pyrene levels (300 to 500 ppm) were consistent with an expected dermal carcinogenic response.

4.1.5 Toxicity for Reproduction

Reproductive and Developmental Toxicity

A teratology range-finding study was conducted on Heavy Pyrolysis Fuel Oil (Rerun Tower Bottoms) via whole body inhalation in Sprague-Dawley rats for 6 hr/day at doses of 0, 0.15, 0.74, and 5.1 g/m^3 during days 6 to 15 of the 20 day gestation duration (Rose *et al*., 1984). During exposure, 5.1 g/m^3 females showed closing or partial closing of eyes, inactivity and abnormal body posture. Between exposures, 5.1 g/m^3 females showed lethargy, red staining of snout, slight general vasodilation, and increased urination and staining of urogenital region with occasional signs of slight ataxia and increased salivation. Food consumption was reduced during the treatment period and water consumption was markedly increased during and post-treatment at the high dose while other groups were similar to controls. At 5.1 g/m^3, body weight loss occurred during the first four days of treatment. Body weight gain in the 0.74 g/m^3 group was marginally lower than controls, but regained parity by day 14. From days 14 to 20 of gestation, weight gain in high dose animals improved but did not reach parity with other dose groups. At necropsy, no gross abnormalities were observed in parental animals. The pregnancy rate was 80 to 100% in all groups. The incidence of corpora lutea, implantation, and live young were comparable to or higher in treated groups than controls. At 5.1 g/m^3, mean fetal weight was markedly reduced and mean number of intra-uterine deaths was higher. These effects of lesser magnitude were also observed in the 0.74 g/m^3 group litters. No teratogenic effects (malformations or variations) were observed at necropsy. NOAELs (maternal) of 0.74 g/ m^3 and (developmental) of 0.15g/ m^3 were determined.

A definitive dermal teratology study was conducted on Heavy Pyrolysis Fuel Oil (Rerun Tower Bottoms - RTB) in New Zealand White rabbits at doses of 0, 10, 25, and 50 mg/kg/day during days 6 to 18 of gestation (Spicer and Schardein, 1981). Dermal irritation at application site was observed in all treatment groups with a dose-related increase in number of females exhibiting peeling of the epidermal layer. One 50 mg/kg/day non-gravid female died during gestation, probably the result of respiratory distress. Eight rabbits aborted, one each in proximate controls and 25 mg/kg/day group, 2 in 10 mg/kg/day group, 4 in 50 mg/kg/day group; no abortions occurred in remote control animals. The reason for the high abortion rate may have been a consequence of severe dermal irritation in treated groups and inhalation of vapor may have been a contributing factor. No significant differences in mean maternal or fetal observations at caesarean section or in number of litters with malformations and genetic or developmental variations were identified in treated groups compared to controls. No fetal toxicity was observed. Rerun Tower Bottoms did not produce a teratogenic response at any treatment level. A NOAEL (maternal) was not established due to dermal irritation at all dose levels. A NOAEL (developmental) of 50 mg/kg/day was established.

A 1-generation reproductive toxicity was conducted on EDS Experimental Fuel Oil in Sprague-Dawley rats via oral gavage once a day, 5 days/wk. The study was approximately 142 days (90 days exposure, 10 days mating, 40 to 42 days gestation and lactation) at doses of 0, 0.02, 0.1, and 0.5 g/kg/day diluted in highly refined white oil (McKee *et al*., 1987a). No treatment related mortality or significant differences in body weight gain, food consumption or physical signs, except for urogenital staining in high dose animals were observed. Pregnancy indices were comparable in all dose groups: 81%, 86%, 89%, and 83% in control, low, mid and high dose groups, respectively. No significant differences were observed in length of gestation or in maternal weight gain during

gestation. No treatment related effects were observed in mean litter size, live births or pup survival or in pup body weight throughout lactation to weaning. Coal-derived experimental fuel oil administered orally to male and female rats at doses up to 0.5 g/kg/day for 13 weeks prior to mating did not adversely affect reproductive capacity or performance. There was no treatment-induced effect on overall incidence of abnormalities in any treated group or increased incidence of any specific class of malformations. A NOAEL (maternal) of 0.5 g/kg/day and a NOAEL (offspring) of 0.5 g/kg/day were assigned.

A developmental toxicity study (OECD 414) was conducted on EDS Experimental Fuel Oil in Sprague-Dawley rats via oral gavage on gestational days 6 to 19 at doses of 0, 0.1, 0.5, and 1.0 g/kg/day (McKee *et al*., 1987b). Maternal body weight gain and uterine weight at term were significantly reduced in the middle and high dose groups. There also were increased clinical observations in these groups that included nasal, ocular, oral, and vaginal discharges, rales, and ungroomed appearance. The middle and high dose groups exhibited significant increases in early embryonic resorptions with corresponding decreases in the mean number of live fetuses (86% and 25% compared to 100% in the control and low dose). The remaining fetuses in the 0.5 and 1.0 g/kg/day dose groups had significantly reduced fetal body weight and crown-rump distance. The overall number of fetal skeletal malformations was not significantly different from the controls, although the ratios of malformed fetuses per litter were significantly increased in the middle and high groups. Gross visceral abnormalities were observed only in the middle and high dose groups. Coal-derived experimental fuel oil administered orally to pregnant female rats was embryolethal and teratogenic in rats at doses that are maternally toxic. Under the conditions of this study, the test substance was not a selective developmental toxicant. Based on these results both maternal and developmental NOAELs were determined to be 0.1 g/kg/day.

Conclusion

Adequate in vitro and in vivo rodent data data are available to characterize the teratogenic, reproductive, and developmental toxicity potential of Fuel Oils Category streams for purposes of the HPV program. In these studies no developmental or reproductive toxicity was observed at doses that were not maternally toxic other than occasional slight decrease in fetal body weight. Systemic effects were observed in parental animals including reduced body weight gain and increased clinical observations. Based on available data, Fuel Oils Category streams are unlikely to induce teratogenic, reproductive or developmental toxicity. The data are summarized in Table 14.

Table 14. Summary of Developmental Toxicity Data for the Fuel Oils Category

CAS RN and Substance Name	Test Organism	Test Type	NOAEL
Heavy Pyrolysis Fuel Oil (Rerun Tower Bottoms)	Sprague-Dawley Rat	Inhalation Teratology	Maternal - 0.74 g/m^3 Developmental - 0.15 g/m^3
Heavy Pyrolysis Fuel Oil (Rerun Tower Bottoms)	New Zealand White Rabbit	Dermal Teratology	Maternal - Not Established Developmental - 0.05 g/kg/day**
EDS Experimental Fuel Oil*	Sprague-Dawley Rat	OECD 414 Oral Developmental	Maternal - 0.1 g/kg/day Fetal - 0.1 g/kg/day
EDS Experimental Fuel Oil*	Sprague-Dawley Rat	1-Gen Reproductive	Maternal - 0.5 g/kg/day** Offspring - 0.5 g/kg/day**

* Material of similar composition used as read-across data to support the category.
** NOAEL equal to highest dose tested.

4.2 Assessment Summary for Human Health

Existing *in vitro and in vivo* data are sufficient to characterize the human health hazards of substances included in the Fuel Oils Category for purposes of the HPV program. From data on representative streams, and read-across from streams of similar composition, it can be concluded that Fuel Oils Category streams are not acutely toxic by the oral dermal or inhalation routes of exposure. Streams in the Fuel Oils Category are likely to be irritating to the skin and eyes.

Data are available to adequately characterize the repeated dose toxicity of the Fuel Oils Category. The most consistent observations among the studies were decreased body weight and alterations in certain clinical chemistry and hematology parameters. Dermal irritation and ocular discharge were often noted.

Adequate data are available to characterize the teratogenic, reproductive, and developmental toxicity potential of Fuel Oils Category streams. In these studies no developmental or reproductive toxicity was observed at doses that were not maternally toxic, other than an occasional slight decrease in fetal body weight. Systemic effects were observed in parental animals including reduced body weight gain and increased clinical observations. Based on available data, Fuel Oils Category streams are unlikely to induce teratogenic, reproductive or developmental toxicity at doses below those causing maternal toxicity.

Adequate data are available to characterize the genotoxic potential of Fuel Oils Category streams. The results of a diverse array of mutagenicity, cell transformation, and clastogenicity assays indicate positive responses in some assays and negative responses in others. Light Pyrolysis Fuel Oil, Heavy Pyrolysis Oil and Biphenyl Feedstock demonstrated activity in assays for general genetic damage, unscheduled DNA synthesis and sister chromatid exchange, but were inactive in assays for mutagenicity (HGPRT and Ames assays), clastogenicity (micronucleus) and cell transformation. Aromatic Pyrolysis Oil was determined to be mutagenic and clastogenic, induced DNA synthesis (indication of repair) and produced transformation in culture cells. EDS Experimental Fuel Oil was mutagenic in the Ames assay and transformed Syrian hamster embryo cells in culture. Mutagenic activity required metabolic activation. Using Aromatic Pyrolysis Oil as the most biologically active member of the Fuel Oils Category, it is concluded that these streams are potentially genotoxic.

Limited but adequate data are available to characterize the Fuel Oils Category streams for dermal carcinogenicity potential after repeated dermal exposure. Pyrolysis Fuel Oil was carcinogenic in the mouse skin painting bioassay. Although the method used a qualitative procedure of skin painting rather than exact volume application, and the material was not analyzed, the results were unambiguous. The described process conditions and the benzo(a)pyrene levels (300 to 500 ppm) were consistent with an expected dermal carcinogenic response.

Taken as a whole, these data suggest that the most sensitive health effects for Fuel Oils are due to the high content of polyaromatic and polycyclic hydrocarbons that are present in most of the category streams.

5 HAZARDS TO THE ENVIRONMENT

5.1 Aquatic Toxicity

The aquatic toxicity of streams in this category is expected to fall within a relatively narrow range regardless of their composition. This is expected because the constituent chemicals of these streams are neutral organic hydrocarbons whose toxic mode of action is non-polar narcosis (Ramos *et al.*, 1998). The toxic mechanism of short-term toxicity for these chemicals is disruption of biological membrane function (Van Wezel, 1995), and the differences between toxicities (i.e., LC/LL_{50}, EC/EL_{50}) can be explained by the differences between the target tissue-partitioning behavior of individual constituent chemicals (Verbruggen *et al.*, 2000).

The existing fish toxicity database for hydrophobic, neutral organic chemicals, which compose the streams in this category, supports a critical body residue (CBR) for these chemicals between approximately 2 to 8 mmol/kg fish (wet weight) (McCarty *et al.*, 1991; McCarty and Mackay, 1993). The CBR is the internal concentration of a toxicant that causes mortality. When normalized to lipid content for most organisms, the CBR is approximately 50 umol/g of lipid (Di Toro *et al.*, 2000). Therefore, only hydrocarbon streams with components of sufficient water solubility, such that their molar sum in solution is high enough to produce a total partitioning to the organism of approximately 50 umol of hydrocarbon per gram of lipid, will demonstrate lethality.

Fish, invertebrate, and alga toxicity data are available for two different complex category streams, Heavy Pyrolysis Fuel Oil and Pyrolysis C10+ Fuel Oil. In addition, there are also data available for two analog substances that are not in this category, but are either compositionally similar or are known to contain constituents similar to category members. These two substances are biphenyl feedstock (CAS RN 68989-41-3) and No. 2 fuel oil (CAS RN 68476-30-2). The category member and analog data were applied to characterize the remaining untested streams in this category.

The results for the two tested category members showed relatively narrow effect ranges (Table 15). The 96-hour LC_{50} and LL_{50} results for rainbow trout range between 1.0 to 4.4 and 1.1 to 5.6 mg/L, respectively. The 48-hour EC_{50} and EL_{50} results for a daphnid range between 1.2 to 2.7 and 1.2 to 3.3 mg/L, respectively. The 96-hour EC_{50} and EL_{50} results based on biomass and growth rate for a green alga range from 0.9 to 1.6 and 1.2 to 2.2 mg/L, respectively, while the 96-hour NOEC and NOELR results based on biomass and growth rate range between 0.12 to 0.42 and 0.18 to 0.39 mg/L, respectively.

Table 15. Summary of Aquatic Toxicity Data for Substances in the Fuel Oils Category

CAS RN and Substance Name	Fish Toxicity (*Oncorhynchus mykiss*) 96-hour LC_{50} 96-hour LL_{50} (mg/L)	Invertebrate Toxicity (*Daphnia magna*) 48-hour EC_{50}; 48-hour EL_{50} (mg/L)	Alga Toxicity (*Pseudokirchneriella subcapitata*) 96-hour EC_{50}; 96-hour NOEC - 96-hour EL_{50}; 96-hour NOELR (mg/L)
Heavy Pyrolysis Fuel Oil 68513-69-9, 64741-62-4, 69013-21-4, 8002-05-9	4.4; 5.6 (EMBSI, 2004c)	2.7; 3.3 (EMBSI, 2004d)	1.3b; 0.42b 1.8r; 0.42r - 1.4b; 0.39b 2.1r; 0.39r (EMBSI, 2004e)
Pyrolysis C10+ Fuel Oil 68513-69-9, 68921-67-5	1.0; 1.1 (EMBSI, 2004f)	1.2; 1.2 (EMBSI, 2004g)	0.9b; 0.12b 1.6r; 0.12r - 1.2b; 0.18b 2.2r; 0.18r (EMBSI, 2004h)

b biomass
r growth rate
EMBSI ExxonMobil Biomedical Sciences, Inc.

Studies for the two analog substances include two fish acute studies and a daphnid acute study (Table 16). The endpoints for these studies were reported as either lethal or effect loading (LL and EL) values. Concentration data comparable to the data available for the two category members were not included in these studies. Although the loading results from one fish study with *Menidia beryllina* are consistent with the loading data for the two category members, the results from the second study with *Cyprinodon variegates* are comparably higher. This may be a reflection of differences in sensitivity between species, both *Menidia* and *Cyprinodon* are marine water species in comparison to the studies conducted with the freshwater species, *Oncorhynchus mykiss.*

The analog study with *Daphnia* also provided a loading value that was higher than the results for the two category members (Table 16). However, this was most likely the result of the test procedure, which prepared a stock solution at a loading of 1,000 mg/L and diluted the aqueous phase (water accommodated fraction, WAF) to prepare each of the exposure solutions. In comparison, the exposure solutions for the two category member daphnid studies were prepared by developing separate WAFs of each of the exposure solutions (this is the currently acceptable procedure for complex, poorly water soluble substances). This difference in methodology may have contributed to the higher effect values demonstrated by the biphenyl feedstock.

Table 16. Summary of Aquatic Toxicity Data for Analog Substances Used to Support the Fuel Oils Category

CAS RN and Substance Name	Fish Toxicity (*Cyprinodon variegates*) 96-hour LL_{50} (mg/L)	Fish Toxicity (*Menidia beryllina*) 96-hour LL_{50} (mg/L)	Invertebrate Toxicity (*Daphnia magna*) 48-hour EL_{50} (mg/L)
Biphenyl Feedstock 68989-41-3	-	-	23.6 (Meyers and Rausina, 1984)
No. 2 Fuel Oil 68476-30-2	56.0 (EBSI, 1998a)	3.2 (EBSI, 1998b)	-

b biomass
r growth rate
EMBSI ExxonMobil Biomedical Sciences, Inc.

Two additional aquatic toxicity robust summaries were submitted with the Fuel Oils Category test plan (Olefins Panel, HPV Implementation Task Group, 2003) that were not used in this report. The first summarized an alga toxicity study (Bingman and Rausina, 1983) conducted with biphenyl feedstock (CAS RN 68989-41-3). These data were not used because the study quality was assessed as "invalid". The second summarized an invertebrate toxicity study (EBSI, 1993) conducted with No. 2 fuel oil (CAS RN 68476-30-2). These data were not used because the test procedure did not follow a standard test guideline, and the endpoint is neither conventional nor comparable to any of the other results from toxicity studies described in this report.

5.2 Assessment Summary for the Environment

Results of distribution modeling show that constituents of streams in the Fuel Oils Category will partition largely between the air, water, and soil compartments, with a negligible amount partitioning to sediment. Volatilization to the air can contribute to the loss of some constituents from aqueous and terrestrial habitats. Although some constituents have a moderate degree of water solubility, wet deposition of category constituents is not likely to play a significant role in their atmospheric fate because they rapidly photodegrade. In the air, these constituents have the potential to rapidly degrade through indirect photolytic processes mediated primarily by hydroxyl radicals with calculated degradation half-lives ranging from 1.1 to 53.0 hours, depending on hydroxyl radical concentration. Aqueous photolysis and hydrolysis will not contribute to the transformation of category constituents in aquatic environments because they are either poorly or not susceptible to these reactions. Streams in this category are subject to biodegradative processes. Two category streams, Heavy Pyrolysis Fuel Oil and Pyrolysis C10+ Fuel Oil, and one analog stream, 1,1'-biphenyl, exhibited a range of 7 to 57% biodegradation after 28 days under standard testing procedures. The remaining streams that were not tested are expected to demonstrate a similar range of biodegradability.

Aquatic toxicity testing results for two different complex streams, Heavy Pyrolysis Fuel Oil and Pyrolysis C10+ Fuel Oil, suggest that category members will exhibit a moderate order of toxicity. The effect values for the two streams fell within a relatively narrow range. The two streams combined, contain constituents shared by the remainder of the streams within this category, and therefore justifies their use to characterize the potential effects of the untested streams.

The 96-hour LC_{50} and LL_{50} results for *Oncorhynchus mykiss* (rainbow trout) range between 1.0 to 4.4 and 1.1 to 5.6 mg/L, respectively. The 48-hour EC_{50} and EL_{50} results for *Daphnia magna* (invertebrate) ranged between 1.2 to 2.7 and 1.2 to 3.3 mg/L, respectively. The 96-hour EC_{50} and

EL_{50} results based on biomass and growth rate for *Pseudokirchneriella subcapitata* (green alga) range from 0.9 to 1.6 and 1.2 to 2.2 mg/L, respectively, while the 96-hour NOEC and NOELR results based on biomass and growth rate range between 0.12 to 0.42 and 0.18 to 0.39 mg/L, respectively. Fish acute toxicity data (96-hour LL_{50}) for two marine species that were developed with an analog substance and only reported as lethal loading values were 3.2 and 56.0 mg/L. A second analog substance tested in an acute *Daphnia magna* study exhibited a 48-hour EL_{50} = 23.6 mg/L. Untested streams are expected to exhibit toxicities within the range of values demonstrated by these data.

6 DATA SUMMARY

Physico-chemical, environmental fate and effects, and human health data that characterize the 8 streams in the Fuel Oils Category are summarized in Tables 17 and 18. CAS RNs are associated with streams as follows:

- **Heavy Pyrolysis Fuel Oil**
  - 68513-69-9
  - 64741-62-4
  - 69013-21-4
  - 8002-05-9
- **Quench Oil Combined**
  - 68513-69-9
  - 69430-33-7
- **Light Pyrolysis Fuel Oil**
  - 68475-80-9
  - 68514-34-1
  - 68527-18-4
- **Pyrolysis C10+ Fuel Oil**
  - 68513-69-9
  - 68921-67-5
- **Combined Fuel Oil (E&P)**
  - 64742-90-1
  - 68131-05-5
  - 68527-18-4
  - 69013-21-4
- **Hydrotreated Flux Oil**
  - 64742-47-8
  - 69013-21-4
- **Biphenyl Concentrate**
  - 68409-73-4
- **Combined Fuel Oil (B&P)**
  - 68513-69-9

Table 17. Physico-Chemical and Environmental Data Used to Characterize Streams and CAS RNs in the Fuel Oils Category

Endpoint	Fuel Oils (FOs) Category Streams and CAS RNs							
	FO1	**FO2**	**FO3**	**FO4**	**FO5**	**FO6**	**FO7**	**FO8**
	Heavy Pyrolysis FO	**Quench Oil Combined**	**Light Pyrolysis FO**	**Pyrolysis C10+ FO**	**Combined FO (E&P)**	**Hydrotreated Flux Oil**	**Biphenyl Concentrate**	**Combined FO (B&P)**
	68513-69-9, 64741-62-4, 69013-21-4, 8002-05-9	**68513-69-9, 69430-33-7**	**68475-80-9, 68514-34-1, 68527-18-4**	**68513-69-9, 68921-67-5**	**64742-90-1, 68131-05-5, 68527-18-4, 69013-21-4**	**64742-47-8, 69013-21-4**	**68409-73-4**	**68513-69-9**
Boiling Point Range (°C @760 mm Hg)	201 to 340 (m)	114 to 340* (m)		114 to 248 (m)	114 to 340* (m)			
Vapor Pressure Range (hPa @ 25 °C)	2.1 (m)	2.1 to 4.0* (m)		4.0 (m)	2.1 to 4.0* (m)			
Log P_{ow} Range (25 °C)	3.4 to 5.0 (m)	3.3 to 5.4* (m)		3.3 to 5.4 (m)	3.3 to 5.4* (m)			
Melting Point*/ Range (°C)	32.0 to 80.2 (m)							
Water Solubility*/ Range (mg/L @ 25 °C)	29.0 to 142.1 (m)							
Direct Photodegradation	Direct photolysis will not contribute to degradation							
Indirect (OH-) Photodegradation* (half-life, hrs) (c)	1.1 to 53.0 (a)							
Hydrolysis	Hydrolysis will not contribute to degradation							
Distribution*	12 to 99% partitions to air, <1 to 31% partitions to water, 1 to 77% partitions to soil, <2% partitions to sediment							

* Constituent chemicals used to define selected endpoints include: indene, dicyclopentadiene, naphthalene, methylnaphthalene, and 1,1'-biphenyl.
(m) Measured values (c) Calculated values (a) Atmospheric half-life values are based on a 12-hr day.

Table 17. Continued

Endpoint	Fuel Oils (FOs) Category Streams and CAS RNs							
	FO1	**FO2**	**FO3**	**FO4**	**FO5**	**FO6**	**FO7**	**FO8**
	Heavy Pyrolysis FO	**Quench Oil Combined**	**Light Pyrolysis FO**	**Pyrolysis C10+ FO**	**Combined FO (E&P)**	**Hydrotreated Flux Oil**	**Biphenyl Concentrate**	**Combined FO (B&P)**
	68513-69-9, 64741-62-4, 69013-21-4, 8002-05-9	**68513-69-9, 69430-33-7**	**68475-80-9, 68514-34-1, 68527-18-4**	**68513-69-9, 68921-67-5**	**64742-90-1, 68131-05-5, 68527-18-4, 69013-21-4**	**64742-47-8, 69013-21-4**	**68409-73-4**	**68513-69-9**
Biodegradation (% after 28 days)	29.0	7.3 to 29.0		7.3	7.3 to 29.0		7.3 to 57.0**	
96-hr Fish LC_{50}; LL_{50} (mg/L)	4.4; 5.6	1.0 to 4.0; 1.1 to 56.0**		1.0; 1.1	1.0 to 4.0; 1.1 to 56.0**			
48-hr Invertebrate EC_{50}; EL_{50} (mg/L)	2.7; 3.3	1.2 to 2.7; 1.2 to 23.6**		1.2; 1.2	1.2 to 2.7; 1.2 to 23.6**			
96-hr Alga EC_{50}; EL_{50} (mg/L)	1.3; 1.4b 1.8; 2.1r	0.9 to 1.3; 1.2 to 1.4b 1.6 to 1.8; 2.1 to 2.2r		0.9; 1.2b 1.6; 2.2r	0.9 to 1.3; 1.2 to 1.4b 1.6 to 1.8; 2.1 to 2.2r			
96-hr Alga NOEC; NOELR (mg/L)	0.42; 0.39b 0.42; 0.39r	0.12 to 0.42; 0.18 to 0.39b 0.12 to 0.42; 0.18 to 0.39r		0.12; 0.18b 0.12; 0.18r	0.12 to 0.42; 0.18 to 0.39b 0.12 to 0.42; 0.18 to 0.39r			

** Range includes analog data
b biomass
r growth rate

Table 18. Human Health Data Summary Used to Characterize Streams and CAS RNs in the Fuel Oils Category

Endpoint	Human Health Data for Fuel Oils (FOs) Category Streams (CAS RNs)							
	FO1	**FO2**	**FO3**	**FO4**	**FO5**	**FO6**	**FO7**	**FO8**
	Heavy Pyrolysis FO**	**Quench Oil**	**Light Pyrolysis FO**	**Pyrolysis C10+ FO****	**Combined FO (E&P)**	**Hydrotreated Flux Oil****	**Biphenyl Concentrate****	**Combined FO (B&P)**
	68513-69-9, 64741-62-4, 69013-21-4, 8002-05-9	**68513-69-9, 69430-33-7**	**68475-80-9, 68514-34-1, 68527-18-4**	**68513-69-9, 68921-67-5**	**64742-90-1, 68131-05-5, 68527-18-4, 69013-21-4**	**64742-47-8, 69013-21-4**	**68409-73-4**	**68513-69-9**
Acute Toxicity (oral, rat)	14.5 g/kg	≥2.89 g/kg (RA FO3)	2.89 g/kg	≥2.89 g/kg (RA FO3)	>5 g/kg	>5 g/kg	3.7 g/kg	≥2.89 g/kg (RA FO3)
Acute Toxicity (dermal, rabbit)	>5 g/kg	>2 g/kg (RA FO7)				>3.16 g/kg	>2 g/kg	>2 g/kg (RA FO7)
Acute Toxicity (inhalation, rat)	~6.0 g/m^3	>3 g/m^3 (RA FO7)	>4.95 g/m^3	>3 g/m^3 (RA FO7)	>3.7 g/m^3	>3 g/m^3 (RA FO7)	>3 g/m^3	>3 g/m^3 (RA FO7)
Repeat Dose Toxicity (oral; NOAEL, rat)	≥0.1g/kg/d (90 d; RA from FO6)					0.1g/kg/d (90 d)	≥0.1g/kg/d (90 d; RA FO6)	
Repeat Dose Toxicity (dermal; LOEL, rabbit)	≥0.05 g/kg/d (28 d; RA FO6)		1 g/kg/d (8 d; rat)	≥0.05 g/kg/d (28 d; RA FO6)	1 g/kg/d (2 wk; rat)	0.05 g/kg/d (28 d)	1 g/kg/d (12 d)	≥0.05 g/kg/d (28 d; RA FO6)
Repeat Dose Toxicity (inhalation; LOEL, rat)	0.15 g/m^3 (12 d)	0.15 g/m^3 (12 d; RA FO1)	0.51 g/m^3 (28 d)	0.15 g/m^3 (12 d; RA FO1)	0.54 g/m^3 (12 d)	0.15 g/m^3 (12 d; RA FO1)	1.07 g/m^3 (12 d)	0.15 g/m^3 (12 d; RA FO1)
Mutagenicity *in vitro*	Positive (SCE) Negative (Ames)	Positive (RA FO1,3,5,6,7)	Positive (UDS) Negative (CHO; BALB/3T3)	Positive (RA FO1,3,5,6,7)	Positive (CHO; UDS; BALB/3T3)	Positive (SHE; Ames)	Positive (UDS) Negative (CHO; BALB/3T3)	Positive (RA FO1,3,5,6,7)
Mutagenicity *in vivo*	Positive (RA FO5)		Negative (MN)	Positive (RA FO5)	Positive (MN)	Positive (RA FO5)	Negative (MN)	Positive (RA FO5)
Carcinogenicity	Positive (RA FO2)	Positive (dermal, mouse)	Positive (RA FO2)					
Reproductive Toxicity (oral)	≥0.5 g/kg/d (RA FO6)					0.5 g/kg/d	≥0.5 g/kg/d (RA FO6)	
Developmental Toxicity (NOAEL)	0.15 g/m3 (inhal) 0.05 g/kg/d (derm)	≥0.05 g/kg/d (derm; RA FO1)				0.1 g/kg/d (oral)	≥0.05 g/kg/d (derm; RA FO1)	

** Analog data **RA** Read-across data from indicated Fuel Oil (FO) Category stream number

CHO - Chinese Hamster Ovary; **UDS** - Unscheduled DNA Synthesis; **SHE** - Syrian Hamster Embryo; **SCE** - Sister Chromatid Exchange; **BALB/3T3** - Mouse Embryo Cell Transformation Assay; Ames - Ames Salmonella Mutagenicity Assay; **MN** - Mammalian Bone Marrow Erythrocyte Micronucleus

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APPENDIX I

ETHYLENE PROCESS DESCRIPTION

A. Ethylene Process

1. Steam Cracking

Steam cracking is the predominant process used to produce ethylene. Various hydrocarbon feedstocks are used in the production of ethylene by steam cracking, including ethane, propane, butane, and liquid petroleum fractions such as condensate, naphtha, and gas oils. The feedstocks are normally saturated hydrocarbons but may contain minor amounts of unsaturated hydrocarbons. These feedstocks are charged to the coils of a cracking furnace. Heat is transferred through the metal walls of the coils to the feedstock from hot flue gas, which is generated by combustion of fuels in the furnace firebox. The outlet of the cracking coil is usually maintained at relatively low pressure in order to obtain good yields to the desired products. Steam is also added to the coil and serves as a diluent to improve yields and to control coke formation. This step of the ethylene process is commonly referred to as "steam cracking" or simply "cracking" and the furnaces are frequently referred to as "crackers".

Subjecting the feedstocks to high temperatures in this manner results in the partial conversion of the feedstock to olefins. In the simplest example, feedstock ethane is partially converted to ethylene and hydrogen. Similarly, propane, butane, or the hydrocarbon compounds that are associated with the liquid feedstocks are also converted to ethylene. Other valuable hydrocarbon products are also formed, including other olefins, diolefins, aromatics, paraffins, and lesser amounts of acetylenes. These other hydrocarbon products include compounds with two or more carbon atoms per molecule, i.e., C2, C3, C4, etc. Propane and propylene are examples of C3 hydrocarbons and benzene, hexene, and cyclohexane are a few examples of the C6 hydrocarbons.

2. Refinery Gas Separation

Ethylene and propylene are also produced by separation of these olefins streams, such as from the light ends product of a catalytic cracking process. This separation is similar to that used in steam crackers, and in some cases both refinery gas streams and steam cracking furnace effluents are combined and processed in a single finishing section. These refinery gas streams differ from cracked gas in that the refinery streams have a much narrower carbon number distribution, predominantly C2 and/or C3. Thus the finishing of these refinery gas streams yields primary ethylene and ethane, and/or propylene and propane.

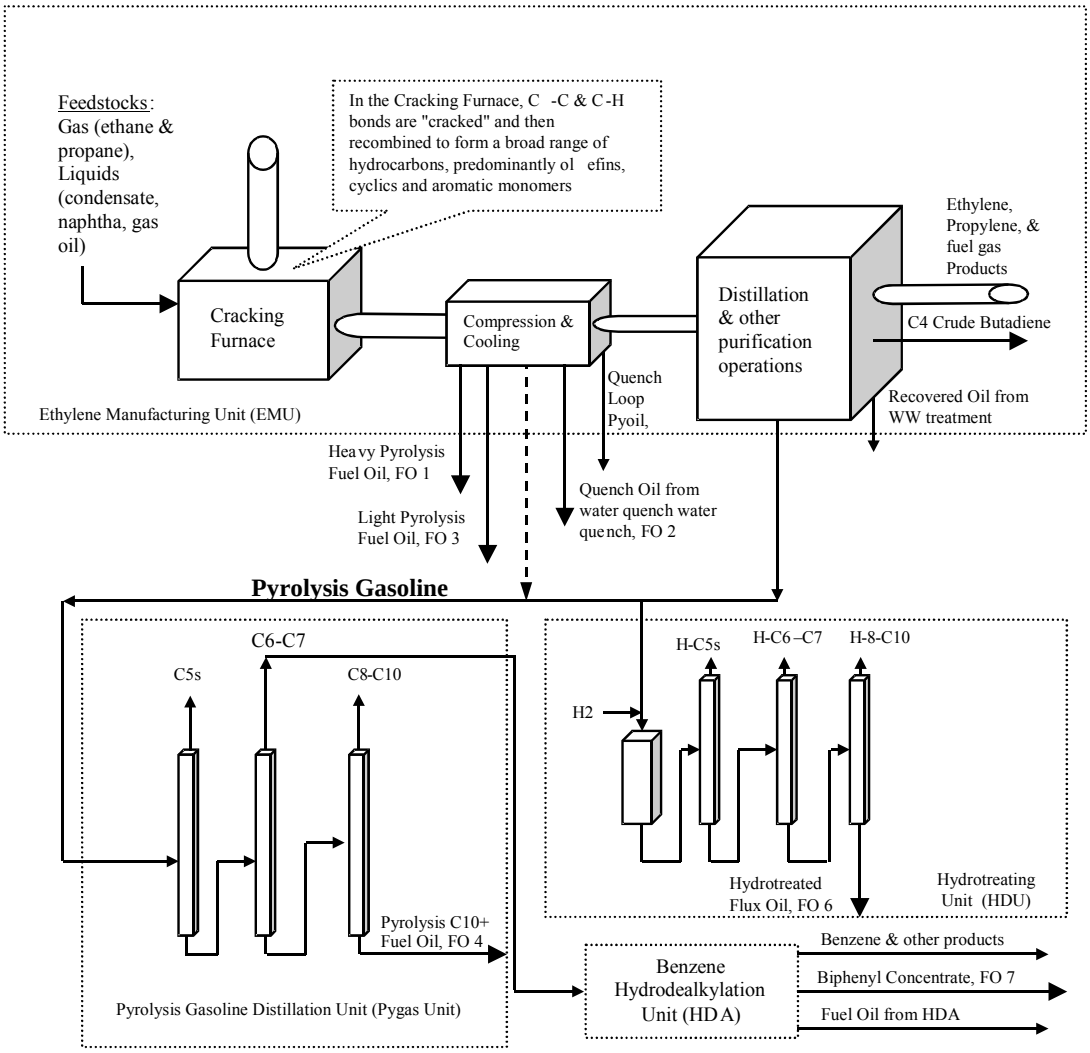
B. Products of the Ethylene Process

The intermediate stream that exits the cracking furnaces (i.e., the furnace effluent) is forwarded to the finishing section of the ethylene plant. The furnace effluent is commonly referred to as "cracked gas" and consists of a mixture of hydrogen, methane, and various hydrocarbon compounds with two or more carbon atoms per molecule (C2+). The relative amount of each component in the cracked gas varies depending on what feedstocks are cracked and cracking process variables. Cracked gas may also contain relatively small concentrations of organic sulfur compounds that were present as impurities in the feedstock or were added to the feedstock to control coke formation. The cracked gas stream is cooled, compressed and then separated into the individual streams of the ethylene process. These streams can be sold commercially and/or put into further steps of the process to produce additional materials. In some ethylene processes, a liquid fuel oil product is produced when the cracked gas is initially cooled. The ethylene process is a closed process and the products are contained in pressure systems.

The final products of the ethylene process include hydrogen, methane (frequently used as fuel), and the high purity products ethylene and propylene. Other products of the ethylene process are typically mixed streams that are isolated by distillation according to boiling point ranges. It is a

subset of these mixed streams that make up the constituents of the Fuel Oils Category. The chemical process operations that are associated with the process streams in the Fuel Oils Category are shown in Figure 4.

Figure 4. Fuel Oils Process Streams Flow Diagram from the Ethylene Manufacturing Process Unit ("FO" or Fuel Oil numbers are used to identify and reference category streams within this document)



Pygas Units are operated in various modes within the industry. Shown above is one arrangement. The Pyrolysis C10+ Fuel Oil (FO 4) is the distillation residue fr om these process arrangements.

If the Pyrolysis Gasoline is hydrotreated prior to distillation, a similar distillation sequence produces a hydrotreated fraction, the Hydrotreated Flux Oil, FO 6.

Frequently the Industry fuel oil streams are not isolated as individual streams at process units. For example, one or more of the Fuel oils from the Ethylene Manufacturing Unit may be combined with a) the fuel oil from the Pygas Unit, yielding the " **Combined Fuel Oil from EMU and Pygas Unit (FO 5),** or b) with the fuel oil from the HDA, yielding the **"Combined Fuel oil from Benzene HDA and EMU, FO 8**).

HPV Fuel Oil Category

Fuel Oil	Fuel Oil Description
FO 1	Heavy Pyrolysis Fuel Oil
FO 2	Quench Oil from water quench
FO 3	Light Pyrolysis Fuel Oil
FO 4	Pyrolysis C10+ Fuel Oil
FO 5	Combined Fuel Oil from EMU and Pygas Unit
FO 6	Hydrotreated Flux Oil
FO 7	Biphenyl Concentrate
FO 8	Combined Fuel Oil from Benzene HDA and EMU

The streams in this category consist of higher boiling hydrocarbons from several classes (Figure 5) and can range predominantly between carbon number 7 and 13 (Figure 6). Categories sponsored by the Olefins Panel of the American Chemistry Council are listed in Table 19.

Figure 5. Percent Hydrocarbon Type in Streams of the Fuel Oils Category (specific compositional data are not available for the FO 1 stream)

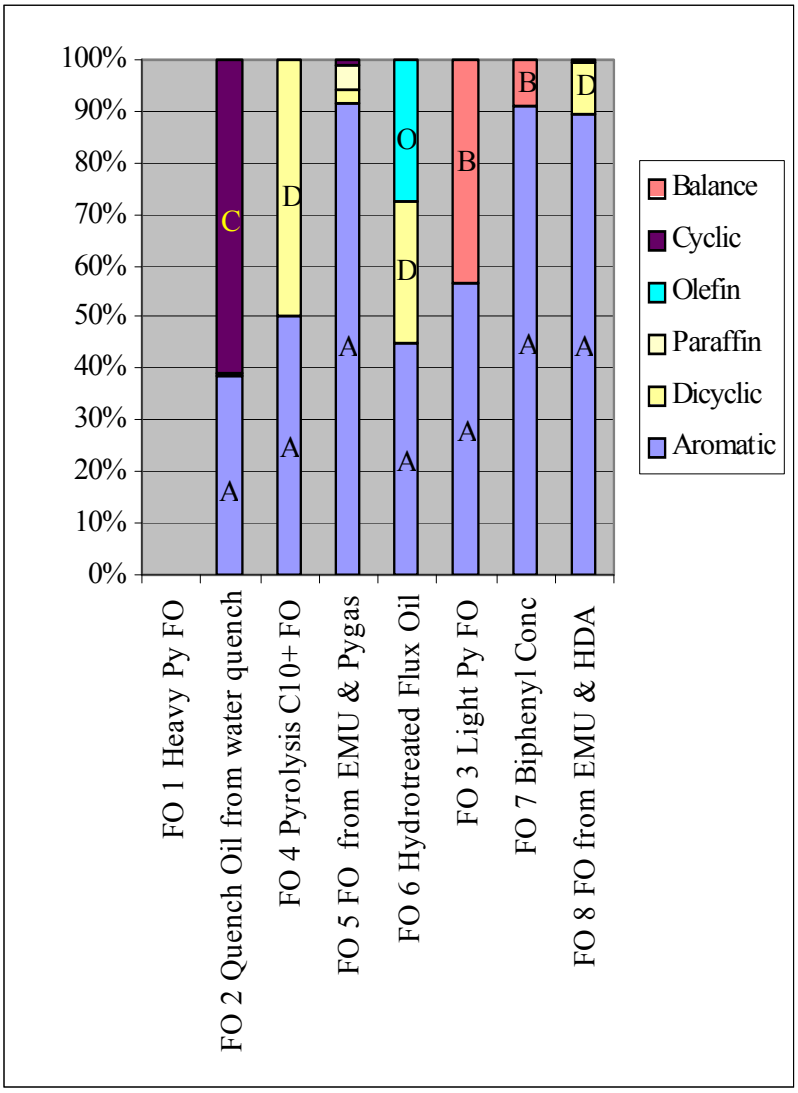


Figure 6. Percent Carbon Number Composition of Streams in the Fuel Oils Category (specific compositional data are not available for the FO 1 stream)

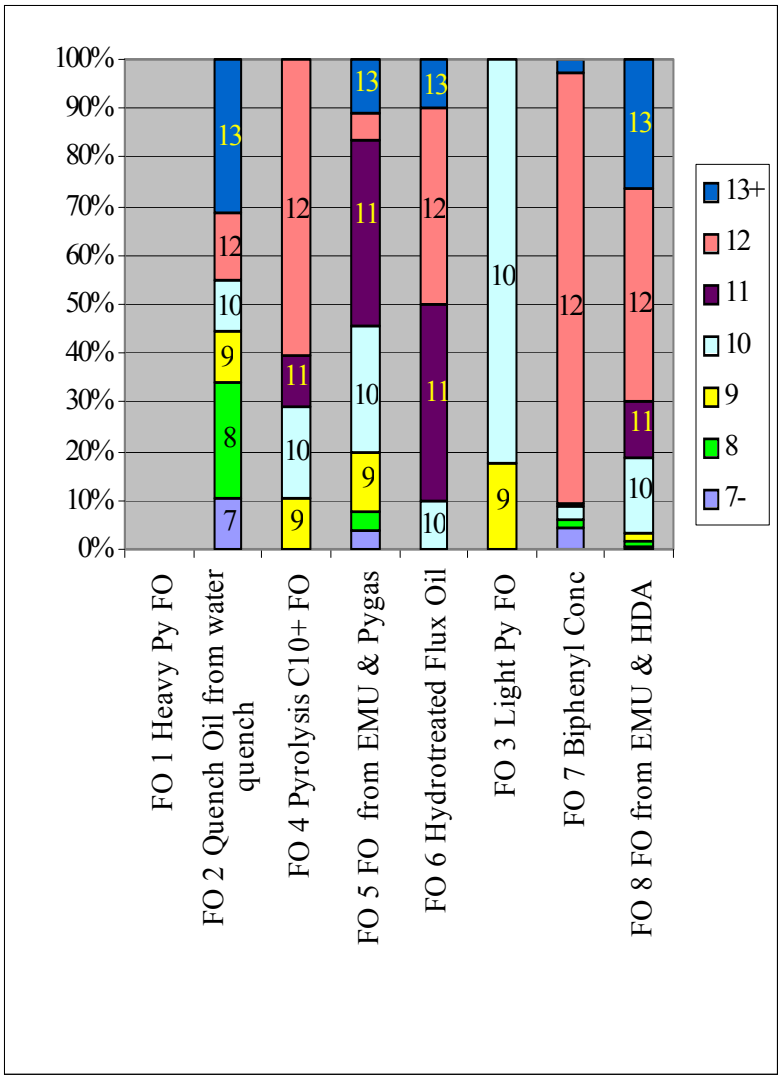


Table 19. HPV Program Categories Sponsored by the Olefins Panel of the American Chemistry Council

Category Number	Category Name
1	Crude Butadiene C4
2	Low 1,3-Butadiene C4
3	C5 Non-cyclics
4	Propylene Streams
5	High Benzene Naphthas
6	Low Benzene Naphthas
7,8,9	Resin Oils & Cyclodiene Dimer Concentrates
10	Fuel Oils
11	Pyrolysis C3+ and Pyrolysis C4+